

VESTA: a three-dimensional visualization system
analysis

Journal of Applied Crystallography

41, 653-658

DOI: 10.1107/s0021889808012016

Citation Report

#	ARTICLE	IF	CITATIONS
1	Determination of the electrostatic potential and electron density of silicon using convergent-beam electron diffraction. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 587-597.	0.3	33
2	Isosymmetrical phase transition in YbV_4O_8 . Acta Crystallographica Section B: Structural Science, 2008, 64, 652-660.	1.8	1
3	Experimental visualization of lithium diffusion in Li_xFePO_4 . Nature Materials, 2008, 7, 707-711.	13.3	647
4	Superconductivity in carrier-doped silicon carbide. Science and Technology of Advanced Materials, 2008, 9, 044204.	2.8	50
5	Origins of band-gap renormalization in degenerately doped semiconductors. Physical Review B, 2008, 78, .	1.1	282
6	Superconductivity Induced by Co-Doping in Quaternary Fluoroarsenide CaFeAsF . Journal of the American Chemical Society, 2008, 130, 14428-14429.	6.6	197
7	Diffusion Path of Oxide Ions in an Apatite-Type Ionic Conductor $\text{La}_{9.69}(\text{Si}_{5.70}\text{Mg}_{0.30})\text{O}_{26.24}$. Chemistry of Materials, 2008, 20, 5203-5208.	3.2	111
8	Structure of $\text{Li}_2\text{FeSiO}_4$. Journal of the American Chemical Society, 2008, 130, 13212-13213.	6.6	254
9	Crystal chemistry and location of hydrogen atoms in prehnite. Mineralogical Magazine, 2008, 72, 1163-1179.	0.6	11
10	Superconductivity in heavily boron-doped silicon carbide. Science and Technology of Advanced Materials, 2008, 9, 044205.	2.8	18
11	Electrochemical Control of the Magnetic Moment of CrO_2 . Journal of the Electrochemical Society, 2008, 155, P83.	1.3	15
12	First-principles studies for structural transitions in ordered phase of cubic approximant Cd_6Ca . Journal of Physics Condensed Matter, 2008, 20, 315206.	0.7	13
13	Columnar magnetic structure coupled with orthorhombic distortion in the antiferromagnetic iron arsenide SrFe_2As_2 . Physical Review B, 2008, 78, .	1.1	60
14	Identification of microscopic spin-polarization coupling in the ferroelectric phase of magnetoelectric multiferroic CuFe . Physical Review B, 2008, 78, .	1.1	35
15	Spin Dynamics in Iron-Based Layered Superconductor $(\text{La}_{0.87}\text{Ca}_{0.13})\text{FePO}_4$ Revealed by ^{51}V and ^{139}La NMR Studies. Physical Review Letters, 2008, 101, 077006.	2.9	47
16	Specific heat and electronic states of superconducting boron-doped silicon carbide. Physical Review B, 2008, 78, .	1.1	43
17	Disorder-order transitions in Na_xMnSi . Physical Review B, 2008, 78, .	1.1	16
18	Disorder-order transitions in MnSi . Physical Review B, 2008, 78, .	1.1	133

#	ARTICLE	IF	CITATIONS
19	First-principles Study of the Bulk Properties for LiMPO ₄ Compounds (M=Mn, Fe, Co, Ni) as Cathode Materials for Lithium Ion Battery. <i>Electrochemistry</i> , 2008, 76, 752-762.	0.6	8
20	Orientalional ordering of three SiO ₄ tetrahedra in $\hat{I}\hat{A}1$ -Ca _{1.5} Sr _{0.5} SiO ₄ that satisfies bond-valence requirements and avoids O-O repulsion. <i>Journal of Mineralogical and Petrological Sciences</i> , 2009, 104, 234-240.	0.4	10
21	Experimental Visualization of Lithium Diffusion in Li _x FePO ₄ . <i>Nihon Kessho Gakkaishi</i> , 2009, 51, 175-181.	0.0	4
22	Elastic properties and electrostructural correlations in ternary scandium-based cubic inverse perovskites: A first-principles study. <i>Physical Review B</i> , 2009, 79, .	1.1	87
23	Comprehensive study on ferroelectricity induced by a proper-screw-type magnetic ordering in multiferroic CuFeO ₂ : Nonmagnetic impurity effect on magnetic and ferroelectric order. <i>Physical Review B</i> , 2009, 79, .	1.1	68
24	Suppression of the mass enhancement in CaCu ₃ Ru ₄ O ₁₂ . <i>Physical Review B</i> , 2009, 80, .	1.1	19
25	Diffuse and doubly split atom occupation in hexagonal LiBH ₄ . <i>Applied Physics Letters</i> , 2009, 95, .	1.5	43
26	Critical behavior of the metallic triangular-lattice Heisenberg antiferromagnet $\langle \text{PdCrO} \rangle^2$ <i>Physical Review B</i> , 2009, 79, .	1.1	69
27	Electronic structure and magnetic properties of monoclinic $\langle \text{Cu} \rangle^2$ <i>Physical Review B</i> , 2009, 79, .	1.1	28
28	Intrinsic exchange bias in $\langle \text{Zn} \rangle^x$ <i>Physical Review B</i> , 2009, 80, .	1.1	30
29	Submillimeter and millimeter wave ESR measurements of frustrated triangular lattice substance InMnO_3 , 2009, , .		0
30	Y ^{4f} O hybridization in the ferroelectric transition of YMnO ₃ . <i>Applied Physics Letters</i> , 2009, 95, .	1.5	44
31	Hydrothermal Synthesis of a New Double Perovskite-Type Bismuthate, (Ba _{0.75} K _{0.14} H _{0.11})BiO ₃ ·nH ₂ O. <i>Japanese Journal of Applied Physics</i> , 2009, 48, 010216.	0.8	25
32	Comparison of crystal structures and the effects of Co substitution in a new member of the Fe-1111 superconductor family AeFeAsF (Ae = Ca and Sr): a possible candidate for a higher- <i>T_c</i> superconductor. <i>Superconductor Science and Technology</i> , 2009, 22, 055016.	1.8	35
33	An NMR study on the F-doping evolution of the iron oxypnictide $\text{LaFeAs}(\text{O}_{1-x}\text{F}_x)$. <i>New Journal of Physics</i> , 2009, 11, 045004.	1.2	33
34	Computational simulations of the structure of Japan twin boundaries in quartz. <i>European Journal of Mineralogy</i> , 2009, 21, 373-383.	0.4	8
35	Thermoelectric properties of Ba ₃ Co ₂ O ₆ (CO ₃) _{0.7} containing one-dimensional CoO ₆ octahedral columns. <i>Journal of Applied Physics</i> , 2009, 106, 034905.	1.1	10
36	Magnetic-Field-Induced Magnetic Phase Transitions Associated with Ferroelectricity in Multiferroic ErMn ₂ O ₅ . <i>Journal of the Physical Society of Japan</i> , 2009, 78, 034718.	0.7	6

#	ARTICLE	IF	CITATIONS
37	Visualizing Rattling in $\text{PrO}_4\text{Sb}_{12}$ by Single Crystal Neutron Diffraction and Maximum-Entropy Analysis. <i>Journal of the Physical Society of Japan</i> , 2009, 78, 074710.	0.7	24
38	A GGA+ <i>U</i> study of the reduction of ceria surfaces and their partial reoxidation through NO_2 adsorption. <i>Molecular Simulation</i> , 2009, 35, 577-583.	0.9	31
39	<i>Ab initio</i> calculations of the structure and mechanical properties of vanadium oxides. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 145404.	0.7	45
40	Heavy-Mass Behavior of Ordered Perovskites $\text{ACu}_3\text{Ru}_4\text{O}_{12}$ (<i>A</i> = Na, Ca, La). <i>Journal of the Physical Society of Japan</i> , 2009, 78, 024706.	0.7	43
41	Adsorption and Reaction Behaviors of Hf Precursor with Two Hydroxyls on Si(100): First Principles Study. <i>Materials Research Society Symposia Proceedings</i> , 2009, 1155, 1.	0.1	1
42	Interaction of Hf Precursor with H ₂ O-terminated Si(001): First Principles Study. <i>Materials Research Society Symposia Proceedings</i> , 2009, 1155, 1.	0.1	0
43	Chemical synthesis and structural characterization of the substitution compound $\text{LaFe}_{1-x}\text{Cu}_x\text{O}_3$ ($x=0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$)	2.0	43
44	Preparation and crystal structure of a new tin titanate containing Sn^{2+} ; Sn_2TiO_4 . <i>Materials Research Bulletin</i> , 2009, 44, 1298-1300.	2.7	33
45	The Effect of Platinum on Diffusion Kinetics in Pt/NiAl : Implications for Thermal Barrier Coating Lifetimes. <i>ChemPhysChem</i> , 2009, 10, 226-235.	1.0	12
46	Density functional and dynamics study of the dissociative adsorption of hydrogen on Mg (0001) surface. <i>Surface Science</i> , 2009, 603, 304-310.	0.8	29
47	Analysis on experimental valence charge density in germanium at RT and 200K. <i>Journal of Physics and Chemistry of Solids</i> , 2009, 70, 1185-1194.	1.9	6
48	$[\text{Zr}_{0.72}\text{Y}_{0.28}]\text{Al}_4\text{C}_4$: A new member of the homologous series $(\text{MC})_l(\text{T}_4\text{C}_3)_m$ ($\text{M}=\text{Zr}, \text{Y}$ and Hf , $\text{T}=\text{Al}, \text{Si}$ and Ge)	1.4	6
49	$\text{Cu}_9\text{Bi}_9\text{S}_{16}\text{Cl}_8$ und $\text{Cu}_{7.4}\text{Bi}_6\text{Se}_{12}\text{Cl}_7$ – Polyedernetzwerke mit Dichalkogenidbrücken und mobilen Kupfer(I)-Kationen. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009, 635, 2162-2169.	0.6	10
50	DFT study on the electronic structure of C_{120} isomers derived from the general Stone-Wales rearrangement. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2773-2779.	1.0	1
51	$\text{Eu}_3\text{Si}_{15}\text{Al}_2\text{O}_{12}$ (f^5) as a commensurate composite crystal. <i>Acta Crystallographica Section B: Structural Science</i> , 2009, 65, 567-575.	1.8	12
52	PeckCryst: a program for structure determination from powder diffraction data using a particle swarm optimization algorithm. <i>Journal of Applied Crystallography</i> , 2009, 42, 1189-1193.	1.9	8
53	Crystal structure of $\text{UO}_2\text{SO}_4 \cdot 2.5\text{H}_2\text{O}$: Full anisotropic refinement and vibration characteristics. <i>Journal of Molecular Structure</i> , 2009, 936, 75-79.	1.8	8
54	Structure and adhesion of MoSi_2/Ni interfaces: Evaluation of MoSi_2 as an alternative bond coat alloy. <i>Surface Science</i> , 2009, 603, 1276-1283.	0.8	3

#	ARTICLE	IF	CITATIONS
55	DFT study of CO and NO adsorption on low index and stepped surfaces of gold. <i>Surface Science</i> , 2009, 603, 2734-2741.	0.8	77
56	Intercalation of Al into MC (M= Ti, V, Cr). <i>Journal of the European Ceramic Society</i> , 2009, 29, 2885-2891.	2.8	11
57	Electric polarization memory effect in a magnetoelectric multiferroic $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$. <i>Physica B: Condensed Matter</i> , 2009, 404, 2532-2534.	1.3	12
58	Effect of intervening structure between CuO_2 sheets in heavily Fe-substituted high- T_c superconductor $\text{FeSr}_2\text{YCu}_2\text{O}_{6+\delta}$. <i>Physica C: Superconductivity and Its Applications</i> , 2009, 469, 960-964.	0.6	0
59	Evaluation of melting point of UO_2 by molecular dynamics simulation. <i>Journal of Nuclear Materials</i> , 2009, 389, 149-154.	1.3	41
60	Synthesis, crystal structure and characterization of iron pyroborate ($\text{Fe}_2\text{B}_2\text{O}_5$) single crystals. <i>Journal of Solid State Chemistry</i> , 2009, 182, 2004-2009.	1.4	19
61	First discovery and structural characterization of a new compound in Al_2SiO_5 system. <i>Journal of Solid State Chemistry</i> , 2009, 182, 2252-2260.	1.4	14
62	Neutron powder diffraction and difference maximum entropy method analysis of protium- and deuterium-dissolved $\text{BaSn}_{0.5}\text{In}_{0.5}\text{O}_{2.75\pm\delta}$. <i>Journal of Solid State Chemistry</i> , 2009, 182, 2632-2639.	1.4	8
63	Crystal structure and electron density in the apatite-type ionic conductor $\text{La}_{9.71}(\text{Si}_{5.81}\text{Mg}_{0.18})\text{O}_{26.37}$. <i>Journal of Solid State Chemistry</i> , 2009, 182, 2846-2851.	1.4	35
64	Synthesis and crystal structure of layered silicate PLS-3 and PLS-4 as a topotactic zeolite precursor. <i>Journal of Materials Chemistry</i> , 2009, 19, 5518.	6.7	64
65	First-principles study on defect chemistry and migration of oxide ions in ceria doped with rare-earth cations. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3241.	1.3	224
66	Universal spectrochemical series of six-coordinate octahedral metal complexes for modifying the ligand field splitting. <i>Dalton Transactions</i> , 2009, , 680-687.	1.6	38
67	Structural Disorder, Diffusion Pathway of Mobile Oxide Ions, and Crystal Structure in Perovskite-Type Oxides and Related Materials. <i>Fuel Cells and Hydrogen Energy</i> , 2009, , 117-145.	0.6	7
68	Tuning Electronic Properties of Hydro-Boron ⁺ Carbon Compounds by Hydrogen and Boron Contents: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18468-18472.	1.5	39
69	Crystal Structures of the Tetragonal Ceria ⁺ Zirconia Solid Solutions $\text{Ce}_{1-x}\text{Zr}_x\text{O}_{2+x}$ through First Principles Calculations ($0 \leq x \leq 1$). <i>Journal of Physical Chemistry C</i> , 2009, 113, 12658-12662.	1.5	30
70	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. <i>Chemistry of Materials</i> , 2009, 21, 5119-5124.	3.2	90
71	Crystal Structure of Tubular Na ⁺ LTA Zeolite Membrane Used for a Vapor Permeation Process: Unusual Distribution of Adsorbed Water Molecules. <i>Industrial & Engineering Chemistry Research</i> , 2009, 48, 10870-10876.	1.8	14
72	Order ⁺ disorder and displacive components in the ferroelectric ⁺ paraelectric phase transition of potassium titanyl phosphate KTiOPO_4 . <i>Chemical Communications</i> , 2009, , 1070.	2.2	15

#	ARTICLE	IF	CITATIONS
73	Kinetic Control of Intralayer Cobalt Coordination in Layered Hydroxides: $\text{Co}_{1-x}\text{Ni}_x\text{O}_{0.5}\text{Co}_{1-x}\text{Ni}_x\text{O}_{0.5}\text{Co}_{1-x}\text{Ni}_x\text{O}_{0.5}\text{Co}_{1-x}\text{Ni}_x\text{O}_{0.5}$ (H ₂ O) ₂ (OH) ₂ (Cl) ₂ (NO ₃) ₂ Inorganic Chemistry, 2009, 48, 11017-11023.	1.9	58
74	Structure and dynamics of water on muscovite mica surfaces. Geochimica Et Cosmochimica Acta, 2009, 73, 4100-4110.	1.6	98
75	Crystal structure and luminescence properties of Sr _x Ca _{1-x} AlSiN ₃ :Eu ²⁺ mixed nitride phosphors. Journal of Alloys and Compounds, 2009, 475, 434-439.	2.8	166
76	Synthesis and crystal structure of Ba ₃ Si ₄ C ₂ . Journal of Alloys and Compounds, 2009, 486, 70-73.	2.8	5
77	Blue photoluminescence, greenish-blue afterglow and their Ti-concentration dependence in rare earth-free bazirite-type BaZr _{1-x} Ti _x Si ₃ O ₉ . Optics Express, 2009, 17, 18054.	1.7	31
78	Atomic displacement parameters and structural disorder of oxygen ions in the CexZr1-xO ₂ solid solutions (0.12 ≤ x ≤ 1.0): Possible factors of high catalytic activity of ceria-zirconia catalysts. Applied Physics Letters, 2009, 94, .	1.5	23
79	(Cu ₂ S) ₂ (Sr ₃ Sc ₂ O ₅) ⁿ A Layered, Direct Band Gap, p-Type Transparent Conducting Oxychalcogenide: A Theoretical Analysis.. Chemistry of Materials, 2009, 21, 5435-5442.	3.2	78
80	Origin of electronic and optical trends in ternary $\ln_{1-x}\text{Ga}_x\text{Sb}_{1-x}$ conducting oxides. Physical Review B, 2009, 79, .	1.1	74
81	Probing local structure in the yellow phosphor LaSr ₂ AlO ₅ :Ce ³⁺ , by the maximum entropy method and pair distribution function analysis. Journal of Materials Chemistry, 2009, 19, 8761.	6.7	42
82	Binary Ethanol-Methane Clathrate Hydrate Formation in the System CH ₄ -C ₂ H ₅ OH-H ₂ O: Confirmation of Structure II Hydrate Formation. Journal of Physical Chemistry C, 2009, 113, 12598-12601.	1.5	51
83	Band Edge Electronic Structure of BiVO ₄ : Elucidating the Role of the Bi s and V d Orbitals. Chemistry of Materials, 2009, 21, 547-551.	3.2	624
84	A crystal-chemical investigation of clinozoisite synthesized along the join Ca ₂ Al ₃ Si ₃ O ₁₂ (OH)-Ca ₂ Al ₂ CrSi ₃ O ₁₂ (OH). American Mineralogist, 2009, 94, 1351-1360.	0.9	12
85	Understanding the p-Type Conduction Properties of the Transparent Conducting Oxide CuBO ₂ : A Density Functional Theory Analysis. Chemistry of Materials, 2009, 21, 4568-4576.	3.2	100
86	Compressibility of the high-pressure polymorph of AlOOH to 17 GPa. Mineralogical Magazine, 2009, 73, 479-485.	0.6	20
87	Calculated properties of fully hydrogenated single layers of BN, BC and graphene: Graphane and its BN-containing analogues. Physical Review B, 2009, 80, .	1.1	55
88	Unraveling Atomic Positions in an Oxide Spinel with Two Jahn-Teller Ions: Local Structure Investigation of CuMn ₂ O ₄ . Journal of the American Chemical Society, 2009, 131, 11450-11457.	6.6	115
89	Theoretical investigation of atomic and electronic structures of Ga ₂ Si ₂ O ₇ . Physical Review B, 2009, 80, .	1.1	27
90	Nucleation tendency and crystallizing phase in silicate glasses: A structural aspect. Applied Physics Letters, 2009, 95, .	1.5	19

#	ARTICLE	IF	CITATIONS
91	Crystal Structure, Oxygen Nonstoichiometry and Conduction Path of LaGaO ₃ -Based Oxide-Ion Conductors. <i>Electrochemistry</i> , 2009, 77, 152-154.	0.6	5
92	Crystal and Electronic Structures and High Temperature Protonic Conduction of LaBaGa _{0.95} Mg _{0.05} O ₄ .DELTA.. <i>Electrochemistry</i> , 2009, 77, 158-160.	0.6	7
93	Synthesis of nitrides and silicon carbide using sodium. <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 1021-1027.	0.5	6
94	Hydrothermal synthesis of a new perovskite-type bismuth oxide: Ba _{0.96} Bi _{0.86} O _{2.59} (OH) _{0.41} . <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 214-216.	0.5	17
95	Comparative Study of Charged and Neutral Oxygen Vacancies in Cubic Zirconia from First Principles. <i>Applied Physics Express</i> , 0, 2, 061402.	1.1	11
96	Ordering in Intercalated Ni Atoms and Electron Density Distributions of Layered Compounds Ni _x TiS ₂ . <i>Journal of the Physical Society of Japan</i> , 2009, 78, 104603.	0.7	2
97	Reinvestigation of crystal structure and structural disorder of Ba ₃ MgSi ₂ O ₈ . <i>Powder Diffraction</i> , 2009, 24, 180-184.	0.4	6
98	Stress-induced martensitic transformation in a Ti ₄₅ Zr ₃₈ Al ₁₇ cast rod. <i>Journal of Physics: Conference Series</i> , 2009, 144, 012090.	0.3	1
99	Diffusion pathway of mobile ions and crystal structure of ionic and mixed conductors - A brief review. <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 1055-1059.	0.5	70
100	Electric-field-induced giant strain in Bi _{0.5} Na _{0.5} TiO ₃ -based single crystals: Influence of high-oxygen-pressure annealing. <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 32-36.	0.5	13
101	Synthesis, crystal structure and physical properties of layered cobalt oxide Ca _x CoO ₂ (x= 0.47). <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 42-46.	0.5	15
102	Crystal structure of pseudobrookite-type Mg ₅ Nb ₄ O ₁₅ from 293 to 1117 K. <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 489-493.	0.5	2
103	Crystal structure of an oxygen deficient strontium cobaltate, Sr ₆ Co ₅ O _{14.3} . <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 89-93.	0.5	8
104	Arrangement of La and vacancies in La _{2/3} TiO ₃ predicted by first-principles density functional calculation with cluster expansion and Monte Carlo simulation. <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 911-916.	0.5	17
105	Synthesis of Sr _{0.99} Eu _{0.01} AlSi ₃ from intermetallic precursor. <i>Journal of the Ceramic Society of Japan</i> , 2009, 117, 115-119.	0.5	23
106	Quantitative Analysis of Structural Defect in Silicalite by Rietveld Refinements Using X-ray Powder Diffraction and ²⁹ Si MAS NMR. <i>Bulletin of the Chemical Society of Japan</i> , 2009, 82, 1160-1169.	2.0	18
107	Si-Al distribution in high-pressure CaAl ₄ Si ₂ O ₁₁ phase: A ²⁹ Si and ²⁷ Al NMR study. <i>American Mineralogist</i> , 2009, 94, 1739-1742.	0.9	13
108	SLAVKOVITE, Cu ₁₃ (AsO ₄) ₆ (AsO ₃ OH) ₄ ·23H ₂ O, A NEW MINERAL SPECIES FROM HORNÍ SLAVKOV AND JACHYMOV, CZECH REPUBLIC: DESCRIPTION AND CRYSTAL-STRUCTURE DETERMINATION. <i>Canadian Mineralogist</i> , 2010, 48, 1157-1170.	0.3	5

#	ARTICLE	IF	CITATIONS
109	Electronic structures and stability of Ag-In-Ca surfaces. Journal of Physics: Conference Series, 2010, 226, 012030.	0.3	5
110	Electron density distribution and crystal structure of lithium barium silicate, $\text{Li}_2\text{BaSiO}_4$. Powder Diffraction, 2010, 25, 336-341.	0.4	2
111	New procedure to obtain Bragg-reflection intensities from <code>FULLPROF</code> suite for powder crystal-structure determination using <code>GEST</code> and <code>PECKCRYST</code> programs. Powder Diffraction, 2010, 25, 374-376.	0.4	2
112	Formation of spherulite and metastable phase in stoichiometric $\text{Ba}_2\text{Si}_3\text{O}_8$ glass. Journal of the Ceramic Society of Japan, 2010, 118, 955-958.	0.5	9
113	Modeling and spectral simulation of matrix-isolated molecules by density functional calculations: A case study on formic acid dimer. Journal of Chemical Physics, 2010, 133, 214502.	1.2	12
114	Room temperature ferromagnetic behavior in the hollandite-type titanium oxide. Journal of Applied Physics, 2010, 107, .	1.1	15
115	Chemical Bonding of Li Ions in $\text{Li}_7\text{P}_3\text{S}_{11}$ Crystal. Journal of the Physical Society of Japan, 2010, 79, 65-68.	0.7	4
116	Structure Determination of H-LDS: An Acidified Form of the Layered Silicate K-LDS. Chemistry Letters, 2010, 39, 747-749.	0.7	5
117	Low temperature synthesis of tetragonal BaTiO_3 by using molten salt. Journal of the Ceramic Society of Japan, 2010, 118, 738-740.	0.5	3
118	Microscopic Coexistence of Ferromagnetism and Superconductivity in Single-Crystal UCoGe . Journal of the Physical Society of Japan, 2010, 79, 023707.	0.7	69
119	Preparation and crystal structure of $[\text{enH}_2]_{0.5}[\text{Ho}(\text{HPO}_4)(\text{SO}_4)(\text{H}_2\text{O})]$ (en; ethylenediamine). Journal of the Ceramic Society of Japan, 2010, 118, 236-240.	0.5	0
120	(Fundamentals 4)Analysis of Neutron Diffraction Data by the Rietveld Method and MEM-based Pattern Fitting. Radioisotopes, 2010, 59, 191-200.	0.1	1
121	Crystal and Electronic Structures of $\text{Bi}_4(\text{Ti}, \text{Si})_3\text{O}_{12}$ Ferroelectrics. Funtai Oyobi Fummatsu Yakin/Journal of the Japan Society of Powder and Powder Metallurgy, 2010, 57, 191-197.	0.1	1
122	Direct Space Methods for Powder X-ray Diffraction for Guest-Host Materials: Applications to Cage Occupancies and Guest Distributions in Clathrate Hydrates. Journal of the American Chemical Society, 2010, 132, 524-531.	6.6	190
123	New Lithium Iron Pyrophosphate as 3.5 V Class Cathode Material for Lithium Ion Battery. Journal of the American Chemical Society, 2010, 132, 13596-13597.	6.6	257
124	Oxygen-vacancy-induced Bi^{IV} -domain clamping in ferroelectric $\text{Bi}_4\text{Ti}_3\text{O}_{12}$. Physical Review B, 2010, 81, .	1.1	97
125	High-pressure X-ray diffraction study of $\hat{\mu}\text{-FeOOH}$. Physics and Chemistry of Minerals, 2010, 37, 153-157.	0.3	33
126	Investigation on $\text{Ge}_5\text{Sb}_x\text{Te}_5$ phase-change materials by first-principles method. Applied Physics A: Materials Science and Processing, 2010, 99, 961-964.	1.1	4

#	ARTICLE	IF	CITATIONS
127	The theoretical shear strength of fcc crystals under superimposed triaxial stress. <i>Acta Materialia</i> , 2010, 58, 3117-3123.	3.8	19
128	Thermally-induced and chemically-induced structural changes in layered perovskite-type oxides $\text{Nd}_{2-x}\text{Sr}_x\text{NiO}_4$ ($x = 0, 0.2, 0.4$). <i>Solid State Ionics</i> , 2010, 181, 402-411.	1.3	39
129	Neutron diffraction study of the crystal structure and structural phase transition of $\text{La}_{0.7}\text{Ca}_{0.3-x}\text{Sr}_x\text{CrO}_3$ ($0 \leq x \leq 0.3$). <i>Journal of Solid State Chemistry</i> , 2010, 183, 392-401.	1.4	6
130	Sensitized red luminescence from Ce^{3+} , Mn^{2+} -doped glaserite-type alkaline-earth silicates. <i>Journal of Solid State Chemistry</i> , 2010, 183, 1303-1308.	1.4	23
131	Synthesis and structural characterization of a new aluminum oxycarbonitride, $\text{Al}_5(\text{O}, \text{C}, \text{N})_4$. <i>Journal of Solid State Chemistry</i> , 2010, 183, 2570-2575.	1.4	12
132	Single crystal X-ray analysis of the electronic structure of the thermoelectric material $\text{Sn}_{1-x}\text{Ge}_x\text{Te}$. <i>Indian Journal of Physics</i> , 2010, 84, 1203-1210.	0.9	4
133	Magnetic hyperfine field at Cr site in AgCrO_2 given by Perturbed angular correlations. <i>Hyperfine Interactions</i> , 2010, 197, 123-128.	0.2	4
134	Ion exchanged potassium titanoniobate as photocatalyst under visible light. <i>Journal of Electroceramics</i> , 2010, 24, 110-114.	0.8	12
135	Photoluminescence and thermal stability of yellow-emitting $\text{Sr}^{1-x}\text{SiAlON}:\text{Eu}^{2+}$ phosphor. <i>Journal of Materials Science</i> , 2010, 45, 3198-3203.	1.7	53
136	Theoretical analysis of electronic and structural properties of anhydrous calcium oxalate. <i>Journal of Thermal Analysis and Calorimetry</i> , 2010, 99, 947-955.	2.0	8
137	Theoretical studies of electronic and crystal structure properties of anhydrous mercury oxalate. <i>Journal of Thermal Analysis and Calorimetry</i> , 2010, 101, 499-504.	2.0	8
138	Application of the charge flipping algorithm to the ab initio structure determination of disordered $\text{ZnCl}_2(\text{BzTz})_2$ [$\text{BzTz} = \text{AN}-(5,6\text{-dihydro-4H-1,3-thiazin-2-yl})-2\text{-aminobenzimidazole}$]. <i>Structural Chemistry</i> , 2010, 21, 1021-1025.	1.0	1
139	Synthesis and photoluminescence of $\text{Ca}^{x}(\text{Sn,Ti})^{1-x}\text{Si}^{1-x}\text{O}$ compounds. <i>Materials Research Bulletin</i> , 2010, 45, 367-372.	2.7	13
140	Synthesis, thermal stability, and oxygen intake/release characteristics of $\text{YBa}(\text{Co}_{1-x}\text{Al}_x)_4\text{O}_{7+\delta}$. <i>Materials Research Bulletin</i> , 2010, 45, 1527-1532.	2.7	27
141	Coupling quantum and continuum scales to predict crack tip dislocation nucleation. <i>Scripta Materialia</i> , 2010, 63, 1212-1215.	2.6	37
142	First-principles study of structural and electronic properties of zincblende $\text{Al}_x\text{In}_{1-x}\text{N}$. <i>Solid State Sciences</i> , 2010, 12, 1641-1644.	1.5	7
143	Adsorption of Proline and Glycine on the $\text{TiO}_2(110)$ Surface: A Density Functional Theory Study. <i>ChemPhysChem</i> , 2010, 11, 1053-1061.	1.0	59
144	Role of Water in Directing Diphenylalanine Assembly into Nanotubes and Nanowires. <i>Advanced Materials</i> , 2010, 22, 583-587.	11.1	187

#	ARTICLE	IF	CITATIONS
145	Mn ^{II} (TCNE) _{3/2} (l ₃) _{1/2} – A 3D Network of Structured Organic-Based Magnet and Comparison to a 2D Analog. <i>Advanced Materials</i> , 2010, 22, 2514-2519.	11.1	46
146	Cobalt Coordination and Clustering in $\text{Co}(\text{OH})_2$ Revealed by Synchrotron X-ray Total Scattering. <i>Chemistry - A European Journal</i> , 2010, 16, 9998-10006.	1.7	31
147	Metal-organic interaction probed by First Principles STM simulations. <i>Progress in Surface Science</i> , 2010, 85, 435-459.	3.8	16
148	Single crystal growth of the metallic triangular-lattice antiferromagnet PdCrO ₂ . <i>Journal of Crystal Growth</i> , 2010, 312, 3461-3465.	0.7	32
149	The relevance of the fluorine interactions in the supramolecular structure of a complex constructed from copper(II) hexafluoroacetylacetonate and the 4 ² -(3-pyridyl)-2,2 ⁶ ,2 ³ -terpyridine ligand. Novel C ^F synthons involving the π -system of the terpyridine moieties and those of the hexafluoroacetylacetonate chelate rings. <i>Journal of Fluorine Chemistry</i> , 2010, 131, 510-516.	0.9	9
150	Intervalence charge transfer in perovskite titanates R _{1/2} Na _{1/2} TiO ₃ :Pr ³⁺ (R=La, Gd, Y, Lu). <i>Journal of Luminescence</i> , 2010, 130, 1725-1729.	1.5	38
151	Preparation, crystal structure and photoluminescence of Mn ²⁺ -doped magnesium pyroborates solid solutions, (Mg _{1-x} Mnx)2B ₂ O ₅ . <i>Journal of Luminescence</i> , 2010, 130, 2161-2165.	1.5	16
152	Synthesis and structure analysis of RUB-50, an LEV-type aluminosilicate zeolite. <i>Microporous and Mesoporous Materials</i> , 2010, 128, 150-157.	2.2	19
153	Bis(4-chloroanilinum) trimolybdate – Synthesis and structural studies of a new polymolybdate material. <i>Journal of Molecular Structure</i> , 2010, 965, 131-136.	1.8	4
154	Study of oxygen ion diffusion in (Ba _{0.5} Sr _{0.5})(Co _{0.8} Fe _{0.2})O _{2.33} through in-situ neutron diffractions at 300 and 720K. <i>Physica B: Condensed Matter</i> , 2010, 405, 2091-2096.	1.3	16
155	Antiferromagnetism of perovskite EuZrO ₃ . <i>Journal of Solid State Chemistry</i> , 2010, 183, 168-172.	1.4	38
156	Neutron powder diffraction study of tetragonal Li ₇ La ₃ Hf ₂ O ₁₂ with the garnet-related type structure. <i>Journal of Solid State Chemistry</i> , 2010, 183, 180-185.	1.4	70
157	Synthesis and structural characterization of Al ₄ Si ₄ -homeotypic aluminum silicon oxycarbide, [Al ₄ Si _{0.6}][O _{1.0} C _{2.0}]C. <i>Journal of Solid State Chemistry</i> , 2010, 183, 636-642.	1.4	12
158	Synthesis and structural characterization of Al ₄ Si ₂ C ₅ -homeotypic aluminum silicon oxycarbide, (Al _{6-x} Si _x)(O _y C _{5-y}) (x ^{1/4} 0.8 and y ^{1/4} 1.6). <i>Journal of Solid State Chemistry</i> , 2010, 183, 2183-2189.	1.4	10
159	Superconducting properties of noncentrosymmetric CaR ₂ Si ₃ . <i>Physica C: Superconductivity and Its Applications</i> , 2010, 470, S762-S763.	0.6	11
160	FP-LAPW study of anhydrous cadmium and silver oxalates: electronic structure and electron density topology. <i>Physica B: Condensed Matter</i> , 2010, 405, 3650-3657.	1.3	14
161	Growth and local structure analysis of ZnS nanoparticles. <i>Physica B: Condensed Matter</i> , 2010, 405, 3700-3703.	1.3	18
162	The supramolecular behavior of the polycatenated double-layer coordination polymer [Cd ₂ (isonicotinate) ₄ (pab)(H ₂ O)] _n (pab=1,4-di-4-pyridyl-2,3-diaza-1,3-butadiene). <i>Journal of Molecular Structure</i> , 2010, 983, 76-81.	1.8	6

#	ARTICLE	IF	CITATIONS
163	Cyclosulfamide as a chiral auxiliary: application to efficient asymmetric synthesis (alkylation/aldolization). <i>Tetrahedron: Asymmetry</i> , 2010, 21, 2361-2366.	1.8	26
164	First-principles investigation on the phase stability and chemical bonding of phase-change random alloys. <i>Solid State Communications</i> , 2010, 150, 1375-1377.	0.9	10
165	Effect of Mg substitution on crystal structure and oxide-ion conductivity of apatite-type lanthanum silicates. <i>Solid State Ionics</i> , 2010, 181, 1024-1032.	1.3	21
166	Ionic conductivity of lithium in spinel-type $\text{Li}_4/3\text{Ti}_5/3\text{O}_4 \rightleftharpoons \text{LiMg}_{1/2}\text{Ti}_3/2\text{O}_4$ solid-solution system. <i>Solid State Ionics</i> , 2010, 181, 994-1001.	1.3	30
167	Dilatometry and high-temperature X-ray diffractometry study of $\text{La}_{0.6}\text{Sr}_{0.4}\text{Ti}_{0.1}\text{Fe}_{0.9}\text{O}_{3-\delta}$ and $\text{La}_{0.6}\text{Sr}_{0.4}\text{Ti}_{0.3}\text{Fe}_{0.7}\text{O}_{3-\delta}$ oxygen-permeable membranes. <i>Solid State Ionics</i> , 2010, 181, 1516-1520.	1.3	7
168	Preparation of CaSiO films by chemical vapor deposition. <i>Surface and Coatings Technology</i> , 2010, 205, 2618-2623.	2.2	3
169	First-principles assessment of hydrogen absorption into FeAl and Fe ₃ Si: Towards prevention of steel embrittlement. <i>Acta Materialia</i> , 2010, 58, 638-648.	3.8	46
170	Ab initio study on plane defects in zirconium-hydrogen solid solution and zirconium hydride. <i>Acta Materialia</i> , 2010, 58, 3927-3938.	3.8	103
171	Theoretical investigation of {110} generalized stacking faults and their relation to dislocation behavior in perovskite oxides. <i>Acta Materialia</i> , 2010, 58, 6072-6079.	3.8	40
172	Guest disorder and high pressure behavior of argon hydrates. <i>Chemical Physics Letters</i> , 2010, 485, 104-109.	1.2	14
173	$\text{Mg}_5\text{TiO}_4(\text{BO}_3)_2$. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2010, 66, i92-i94.	0.4	4
174	The structural phase transition in $\text{SrV}_6\text{O}_{11}$. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2010, 66, i99-i102.	0.4	3
175	Magnetic short-range order diffuse scattering in quasicrystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, 384-393.	0.3	3
176	Superspace description of the homologous series $\text{Ca}_2\text{O}_3(\text{ZnO})_m$. <i>Acta Crystallographica Section B: Structural Science</i> , 2010, 66, 117-129.	1.8	16
177	Revision of the structure of $\text{Cs}_2\text{CuSi}_5\text{O}_{12}$ leucite as orthorhombic Pbca . <i>Acta Crystallographica Section B: Structural Science</i> , 2010, 66, 51-59.	1.8	20
178	The nanosilica hazard: another variable entity. <i>Particle and Fibre Toxicology</i> , 2010, 7, 39.	2.8	636
179	$\text{Cu}_7\text{Bi}_6\text{S}_{10}\text{Cl}_5$ - Mobile Copper(I) Cations Inside Dendritic Channels of a Rigid Framework. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2010, 636, 1860-1864.	0.6	9
180	Extended Occupational and Positional Disorder in Pavonite Homologous Copper Bismuth Chalcogenide Halogenides. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2010, 636, 2433-2438.	0.6	14

#	ARTICLE	IF	CITATIONS
181	Origin of high-density hole doping and anisotropic hole transport in a wide gap layered semiconductor LaCuOSe studied by first-principles calculations. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2010, 207, 1636-1641.	0.8	8
182	Subgap states, doping and defect formation energies in amorphous oxide semiconductor InGaZnO_4 studied by density functional theory. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2010, 207, 1698-1703.	0.8	149
183	Synthesis, Crystal Structure, and Photoluminescence of $\text{SrAl}_2\text{SiAlON:Eu}^{2+}$. <i>Journal of the American Ceramic Society</i> , 2010, 93, 465-469.	1.9	33
184	Anisotropic Thermal Diffusivity and Conductivity of La_2O_3 -Doped Strontium Niobate $\text{Sr}_2\text{Nb}_2\text{O}_7$. <i>Journal of the American Ceramic Society</i> , 2010, 93, 1136-1141.	1.9	48
185	Thermal Conductivity of the Rare-Earth Strontium Aluminates. <i>Journal of the American Ceramic Society</i> , 2010, 93, 1457-1460.	1.9	20
186	Crystal chemistry of Mn^{2+} , Sr-rich and REE-bearing piemontite from the Kamisugai mine in the Sambagawa metamorphic belt, Shikoku, Japan. <i>Journal of Mineralogical and Petrological Sciences</i> , 2010, 105, 142-150.	0.4	6
187	Analyses of Magnetic Structures and Nuclear-Density Distribution by the Structure-Refinement and Three-Dimensional Visualization Systems RIETAN-FP-VENUS. <i>Journal of the Vacuum Society of Japan</i> , 2010, 53, 706-712.	0.3	3
188	First Principles Study of Oxygen Vacancies Near Nickel/Zirconia Interface. <i>E-Journal of Surface Science and Nanotechnology</i> , 2010, 8, 93-100.	0.1	6
189	Applications of the three-dimensional visualization system VESTA in mineralogical sciences. <i>Ganseki Kobutsu Kagaku</i> , 2010, 39, 136-145.	0.1	1
190	Structural Study of Trehalose Dihydrate by Neutron and X-ray Diffraction Experiments. <i>Journal of the Physical Society of Japan</i> , 2010, 79, 074608.	0.7	2
191	A temperature-dependent structure study of gem-quality hibonite from Myanmar. <i>Mineralogical Magazine</i> , 2010, 74, 871-885.	0.6	22
192	Effect of Cobalt-Substitution on the Structure and Thermoelectric Properties of Chimney-Ladder Solid Solution $(\text{Mn}_{1-x}\text{Co}_x)\text{Si}^3$ ($x \sim 1.7$). <i>Advances in Science and Technology</i> , 2010, 74, 22-25.	0.2	6
193	Dipotassium dialuminium cyclooctaphosphate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, i49-i50.	0.2	0
194	Electron density distribution and crystal structure of lithium strontium silicate, $\text{Li}_2\text{SrSiO}_4$. <i>Powder Diffraction</i> , 2010, 25, 4-8.	0.4	11
195	Poly[bis($\frac{1}{4}$ -dodecyl sulfato)calcium]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, m749-m749.	0.2	2
196	A ramsayite-type oxide, $\text{Ca}_2\text{Sn}_2\text{Al}_2\text{O}_9$. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, i72-i72.	0.2	4
197	Crystal chemistry of chromian pumpellyite from Osayama, Okayama Prefecture, Japan. <i>American Mineralogist</i> , 2010, 95, 1294-1304.	0.9	7
198	X-ray absorption and luminescence studies of $\text{Ba}_2\text{Ca}(\text{BO}_3)_2:\text{Ce}^{3+}/\text{Na}^+$ phosphors. <i>Journal of Chemical Physics</i> , 2010, 132, 234701.	1.2	11

#	ARTICLE	IF	CITATIONS
199	Antiferromagnetically Spin Polarized Oxygen Observed in Magnetolectric $TbMn_2O_5$. Physical Review Letters, 2010, 105, 087203.		28
200	Defect activation in willemite-type Zn_2GeO_4 by nanocrystallization. Applied Physics Letters, 2010, 97, .	1.5	32
201	Atomic structure of misfit dislocations in nonpolar ZnO/Al_2O_3 heterostructures. Applied Physics Letters, 2010, 97, 121914.	1.5	14
202	Multiscale modeling of the influence of Fe content in a $Si-Cu$ alloy on the size distribution of intermetallic phases and micropores. Journal of Applied Physics, 2010, 107, 061804.	1.1	25
203	Understanding conductivity anomalies in CuI -based delafossite transparent conducting oxides: Theoretical insights. Journal of Chemical Physics, 2010, 132, 024707.	1.2	101
204	Incommensurate spin-density-wave order in quasi-one-dimensional metallic antiferromagnet NaV_2O_7 . Physical Review B, 2010, 81, .	1.1	27
205	A -site doping-induced renormalization of structural transformations in the $PbSc_{0.5}$. Physical Review B, 2010, 81, .	1.1	15
206	Atomic displacements in the charge ice pyrochlore Bi_2O_7 by neutron total scattering. Physical Review B, 2010, 81, .	1.1	52
207	Theoretical study of Schottky-barrier formation at epitaxial rare-earth-metal/semiconductor interfaces. Physical Review B, 2010, 81, .	1.1	37
208	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. Physical Review B, 2010, 81, .	1.1	61
209	Orbital order, stacking defects, and spin fluctuations in the RbO_2 -electron molecular solid. Physical Review B, 2010, 81, .	1.1	23
210	$NaAlSi_3$: Self-doped semimetallic superconductor with free electrons and covalent holes. Physical Review B, 2010, 81, .	1.1	19
211	Transmission electron microscopy and <i>in situ</i> Raman studies of glassy sanbornite: An insight into nucleation trend and its relation to structural variation. Journal of Applied Physics, 2010, 108, .	1.1	14
212	<i>Ab initio</i> study of the low-temperature phases of lithium imide. Physical Review B, 2010, 82, .	1.1	18
213	Total-scattering descriptions of local and cooperative distortions in the oxide spinel $MgAl_2O_4$. Physical Review B, 2010, 82, .	1.1	26
214	Large constriction of lattice constant in epitaxial magnesium oxide thin film: Effect of point defects on lattice constant. Journal of Applied Physics, 2010, 107, 073523.	1.1	25
215	Crystallization of tungstenbronze-type $Ba_2NaNb_5O_{15}$ in high- Nb_2O_5 -content glass: An inelastic light scattering study. Journal of Applied Physics, 2010, 108, 103519.	1.1	10
216	Origin of the giant optical nonlinearity of Sb_2Te_3 phase change materials. Applied Physics Letters, 2010, 97, .	1.5	35

#	ARTICLE	IF	CITATIONS
217	Charge disproportionation associated with spin ordering in delafossite CuFeO seen via resonant x-ray diffraction. <i>Physical Review B</i> , 2010, 81, in the magnetoelectric pyroxenes	1.1	6
218	LiCr_2X_2		

#	ARTICLE	IF	CITATIONS
235	Saneroite: chemical and structural variations of manganese pyroxenoids with hydrogen bonding in the silicate chain. <i>European Journal of Mineralogy</i> , 2010, 22, 393-402.	0.4	10
236	Ardennite, tiragalloite and medaite: structural control of $(As^{5+}, V^{5+}, Si^{4+})O_4$ tetrahedra in silicates. <i>Mineralogical Magazine</i> , 2010, 74, 55-71.	0.6	17
237	Transport properties of the layered Rh oxide $K_0.49RhO_2$. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 115603.	0.7	24
238	Compressional behavior of solid NeHe ₂ up to 90 GPa. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 095401.	0.7	7
239	Anti-Site Defects and Ion Migration in the $LiFe_{0.5}Mn_{0.5}PO_4$ Mixed-Metal Cathode Material. <i>Chemistry of Materials</i> , 2010, 22, 1242-1248.	3.2	140
240	Coulomb-potential-dependent decohesion of Mg δ phases. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 292203.	0.7	20
241	Crystal structure, magnetic properties, and Mössbauer spectroscopy of new layered iron oxyselenide $Nd_2Fe_2O_3Se_2$. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 346003.	0.7	31
242	DFT-Based Theoretical Calculations of Nb- and W-Doped Anatase TiO_2 : Complex Formation between W Dopants and Oxygen Vacancies. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12777-12783.	1.5	32
243	Tuning Topochemical Polymerization of Diacetylenes: A Joint Synthetic, Structural, Photophysical, and Theoretical Study of a Series of Analogues of a Known Reactive Monomer, 1,6-Bis(diphenylamino)-2,4-hexadiyne (THD). <i>Chemistry of Materials</i> , 2010, 22, 3961-3982.	3.2	34
244	Atomic Displacement Parameters of Ceria Doped with Rare-Earth Oxide $Ce_{0.8}R_{0.2}O_{1.9}$ (R = La, Nd, Sm, Gd, Y, and Yb) and Correlation with Oxide-Ion Conductivity. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2385-2392.	1.5	75
245	Superconducting state in YSn_3 . <i>Physical Review B</i> , 2010, 82, .	1.1	26
246	Calculation of model Hamiltonian parameters for $LaMnO_3$ using maximally localized Wannier functions. <i>Physical Review B</i> , 2010, 81, .	1.1	15
247	A Pseudoatom in a Cage: Trimetallofullerene $Y_3@C_{80}$ Mimics $Y_3N@C_{80}$ with Nitrogen Substituted by a Pseudoatom. <i>ACS Nano</i> , 2010, 4, 795-802.	7.3	66
248	Fetuin-A Is a Mineral Carrier Protein: Small Angle Neutron Scattering Provides New Insight on Fetuin-A Controlled Calcification Inhibition. <i>Biophysical Journal</i> , 2010, 99, 3986-3995.	0.2	95
249	Origins of Hole Doping and Relevant Optoelectronic Properties of Wide Gap p-Type Semiconductor, $LaCuOSe$. <i>Journal of the American Chemical Society</i> , 2010, 132, 15060-15067.	6.6	43
250	Giant Magnetoelastic Coupling in a Metallic Helical Metamagnet. <i>Physical Review Letters</i> , 2010, 104, 247202.	2.9	84
251	Field-driven magnetisation steps in $Ca_3Co_2O_6$: A single-crystal neutron-diffraction study. <i>Europhysics Letters</i> , 2010, 90, 67006.	0.7	27
252	Magnetically induced ferromagnetism in Cu_2 . <i>Physical Review B</i> , 2010, 82, .	1.1	20

#	ARTICLE	IF	CITATIONS
253	Direct observation of orbital ordering in the spinel oxide FeCr_2O_4 using convergent-beam electron diffraction. <i>Physical Review B</i> , 2010, 81, .	1.1	40
254	Structures, Phase Transitions, Hydration, and Ionic Conductivity of $\text{Ba}_4\text{Ta}_2\text{O}_9$. <i>Chemistry of Materials</i> , 2010, 22, 532-540.	3.2	40
255	Structure Analysis of Si-Atom Pillared Lamellar Silicates Having Micropore Structure by Powder X-ray Diffraction. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3466-3476.	1.5	45
256	Ab initio study of the structure and chemical bonding of stable $\text{Ge}_3\text{Sb}_2\text{Te}_6$. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1585.	1.3	37
257	$\text{La}_4\text{LiAuO}_8$ and $\text{La}_2\text{BaPdO}_5$: Comparing Two Highly Stable d^8 Square-Planar Oxides. <i>Inorganic Chemistry</i> , 2010, 49, 4670-4680.	1.9	18
258	Synthesis, Crystal Structure Analysis, and Photoluminescence of Ti^{4+} -Doped $\text{Mg}_5\text{SnB}_2\text{O}_{10}$. <i>Chemistry of Materials</i> , 2010, 22, 5937-5944.	3.2	14
259	Structural, Spectroscopic, and Magnetic Characterization of the Coordination Polymers $[\text{M}^{II}(\text{NCS})_2(\text{bpe})_2] \cdot 3\text{H}_2\text{O} \cdot 2\text{C}_2\text{H}_6$ [M = Co, Ni; bpe = 1,2-Bis(4-pyridyl)ethylene]. Two Interpenetrated Porous Networks. <i>Crystal Growth and Design</i> , 2010, 10, 4874-4882.	1.4	14
260	Chemistry-Controlled Structural Relaxation and Enhanced Redox Abilities in Vanadium-Doped Two-Dimensional Semiconductive $\text{TeMo}_5\text{O}_{16}$ Catalyst. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13277-13286.	1.5	1
261	Investigation of Si Atom Migration in the Framework of MSE-Type Zeolite YNU-2. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19641-19648.	1.5	38
262	The multiferroic phase of DyFeO_3 : an ab initio study. <i>New Journal of Physics</i> , 2010, 12, 093026.	1.2	100
263	Toward the Design of Ferromagnetic Molecular Complexes: Magnetostructural Correlations in Ferromagnetic Triply Bridged Dinuclear Cu(II) Compounds Containing Carboxylato and Hydroxo Bridges. <i>Inorganic Chemistry</i> , 2010, 49, 285-294.	1.9	30
264	Characters of the Tetramethylammonium Ion in ZK-4 Zeolites Depending on Their Si/Al Ratios. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12885-12895.	1.5	10
265	Clathrate Hydrates for Ozone Preservation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11430-11435.	1.2	27
266	Coordination-Induced Shifts of Absorption and Binding Energies in the $\text{SrFe}_2\text{Zn}_3\text{O}_{11}$ System. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19822-19829.	1.5	30
267	$\text{CaCu}_3\text{Pt}_4\text{O}_{12}$: The First Perovskite with the B Site Fully Occupied by Pt^{4+} . <i>Inorganic Chemistry</i> , 2010, 49, 6778-6780.	1.9	18
268	Predicting crystal structures ab initio: group 14 nitrides and phosphides. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8620.	1.3	12
269	Remarkable Oxygen Intake/Release Capability of BaYMn_2O_5 : Applications to Oxygen Storage Technologies. <i>Chemistry of Materials</i> , 2010, 22, 3192-3196.	3.2	86
270	Crystal Structure, Diffusion Path, and Oxygen Permeability of a Pr_2NiO_4 -Based Mixed Conductor ($\text{Pr}_{0.9}\text{La}_{0.1}$) $_2(\text{Ni}_{0.74}\text{Cu}_{0.21}\text{Ga}_{0.05})\text{O}_{4+\delta}$. <i>Journal of the American Chemical Society</i> , 2010, 132, 2385-2392.	6.6	130

#	ARTICLE	IF	CITATIONS
271	Stabilisation of Cu ₆ Sn ₅ by Ni in Sn-0.7Cu-0.05Ni lead-free solder alloys. <i>Intermetallics</i> , 2010, 18, 145-149.	1.8	156
272	Synthesis, crystal structure and luminescent properties of titanium(IV)-doped calcium borostannates, CaSn _{1-x} Ti _x (BO ₃) ₂ . <i>Journal of Alloys and Compounds</i> , 2010, 490, 443-447.	2.8	17
273	Study of charge density and crystal structure of (La _{0.75} Sr _{0.25})MnO _{3.00} and (Ba _{0.5} Sr _{0.5})(Co _{0.8} Fe _{0.2})O _{2.33} at 500-900K by in situ synchrotron X-ray diffraction. <i>Journal of Alloys and Compounds</i> , 2010, 491, 527-535.	2.8	36
274	High-pressure synthesis of novel hydrides Mg _{7-x} A _x TiH _{16-x} (A=Li, Na, K; x=0-1.0) and their reversible hydrogen storage properties. <i>Journal of Alloys and Compounds</i> , 2010, 494, 439-445.	2.8	10
275	First principles study of Li-Si crystalline phases: Charge transfer, electronic structure, and lattice vibrations. <i>Journal of Alloys and Compounds</i> , 2010, 496, 25-36.	2.8	165
276	Synthesis, crystal structure and photoluminescence of Eu ²⁺ -SiALON. <i>Journal of Alloys and Compounds</i> , 2010, 504, 579-584.	2.8	51
277	Accurate analysis of noble gas concentrations in small water samples and its application to fluid inclusions in stalagmites. <i>Chemical Geology</i> , 2010, 272, 31-39.	1.4	41
278	A DFT study of polyanion substitution into the Li-ion battery cathode material Li ₂ FeSiO ₄ . <i>Computational Materials Science</i> , 2010, 50, 191-197.	1.4	25
279	Crystal structure of silver metagermanate, Ag ₂ GeO ₃ . <i>Powder Diffraction</i> , 2010, 25, 15-18.	0.4	1
280	Tuning the Hydrogen Storage in Magnesium Alloys. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1982-1986.	2.1	25
281	A ₃ V ₅ O ₁₄ (A = K, Rb, or Tl), New Polar Oxides with a Tetragonal Tungsten Bronze Related Structural Topology: Synthesis, Structure, and Functional Properties. <i>Inorganic Chemistry</i> , 2010, 49, 6986-6993.	1.9	61
282	Effect of Particle Size on Hydrogen Release from Sodium Alanate Nanoparticles. <i>ACS Nano</i> , 2010, 4, 5647-5656.	7.3	85
283	Hydrogen in tungsten: Absorption, diffusion, vacancy trapping, and decohesion. <i>Journal of Materials Research</i> , 2010, 25, 315-327.	1.2	230
284	Hybrid functional study of proper and improper multiferroics. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5405.	1.3	147
285	Elastic and magnetic effects on the infrared phonon spectra of MnF_2 . <i>Physical Review B</i> , 2010, 82, .	1.1	28
286	Top-Seeded Solution Crystal Growth and Functional Properties of a Polar Material Na ₂ TeW ₂ O ₉ . <i>Crystal Growth and Design</i> , 2010, 10, 4091-4095.	1.4	57
287	X-ray Rietveld and 57Fe Mossbauer studies of epidote and piemontite on the join Ca ₂ Al ₂ Fe ₃ +Si ₃ O ₁₂ (OH)-Ca ₂ Al ₂ Mn ₃ +Si ₃ O ₁₂ (OH) formed by hydrothermal synthesis. <i>American Mineralogist</i> , 2010, 95, 1237-1246.	0.9	10
288	Structurally driven metamagnetism in MnP and related MnP . <i>Physical Review B</i> , 2010, 81, .	1.1	63

#	ARTICLE	IF	CITATIONS
289	Silicic Acid Adsorption and Oligomerization at the Ferrihydrite-Water Interface: Interpretation of ATR-IR Spectra Based on a Model Surface Structure. <i>Langmuir</i> , 2010, 26, 3394-3401.	1.6	71
290	Electronic Structures and Optical Properties of 6H- and 3C-SiC Microstructures and Nanostructures from X-ray Absorption Fine Structures, X-ray Excited Optical Luminescence, and Theoretical Studies. <i>Journal of Physical Chemistry C</i> , 2010, 114, 6966-6975.	1.5	32
291	First-principles calculations of Zn K XANES in Ca-deficient hydroxyapatite. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 384213.	0.7	11
292	Electric field dependence of magnetic correlation in magneto-electric multiferroic CuFeAlO_2 . <i>Journal of Physics: Conference Series</i> , 2010, 200, 012139.	0.3	1
293	Correlation between Luminescence Quantum Efficiency and Structural Properties of Vanadate Phosphors with Chained, Dimerized, and Isolated VO_4 Tetrahedra. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5160-5167.	1.5	162
294	Square Coordinated MnO_2 -Units in $\text{BiMn}_7\text{O}_{12}$. <i>Inorganic Chemistry</i> , 2010, 49, 8709-8712.	1.9	10
295	Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds. <i>Physical Review B</i> , 2010, 82, .	1.1	298
296	Crystal Structures and Magnetic Properties of New Europium Melilites $\text{Eu}_2\text{MSi}_2\text{O}_7$ (M = Mg, Mn) and Their Strontium Analogues. <i>Inorganic Chemistry</i> , 2010, 49, 10809-10814.	1.9	34
297	Periodicity, work function and reactivity of graphene on Ru(0001) from first principles. <i>New Journal of Physics</i> , 2010, 12, 043041.	1.2	104
298	Resonant x-ray scattering from the quadrupole moment in YVO_3 . <i>Physical Review B</i> , 2010, 82, .	1.1	6
299	Effects of filling in CoSb_3 . Local structure, band gap, and phonons from first principles. <i>Physical Review B</i> , 2010, 81, .	1.1	6
300	Charge transfer and antiferromagnetic order in the A-site-ordered perovskite $\text{LaCu}_3\text{Fe}_4\text{O}_{12}$. <i>Journal of Materials Chemistry</i> , 2010, 20, 7282.	6.7	34
301	Cobalt Porphyrin Catalyzed Electrochemical Reduction of Carbon Dioxide in Water. 2. Mechanism from First Principles. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10174-10184.	1.1	130
302	Imma perovskite-type oxynitride LaTiO_2N : structure and electron density. <i>Chemical Communications</i> , 2010, 46, 4704.	2.2	63
303	Experimental visualization of covalent bonds and structural disorder in a gallium zinc oxynitride photocatalyst $(\text{Ga}_{1-x}\text{Zn}_x)(\text{N}_{1-x}\text{O}_x)$: origin of visible light absorption. <i>Chemical Communications</i> , 2010, 46, 2379.	2.2	55
304	Electronic Conductivity and Stability of Doped Titania ($\text{Ti}_x\text{M}_{1-x}\text{O}_2$, M = Nb, Ru, and Ta) A Density Functional Theory-Based Comparison. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13162-13167.	1.5	26
305	Charge transfer in FeOCl intercalation compounds and its pressure dependence: An x-ray spectroscopic study. <i>Physical Review B</i> , 2010, 82, .	1.1	33
306	Evidence for a spin singlet state in the intermetallic semiconductor FeGa_3 . <i>Physical Review B</i> , 2010, 82, .	1.1	26

#	ARTICLE	IF	CITATIONS
307	First-principles calculation of the structure and dielectric properties of Bi ₂ Ti ₂ O ₇ . Physical Review B, 2010, 82, .	1.1	18
308	First-principles study of charge-density waves on Cu surfaces covered by In, Pb, and Bi atoms: Analysis of electronic structure and surface phonons. Physical Review B, 2010, 82, .	1.1	1
309	Robust Refinement as Implemented in TOPAS. Materials Science Forum, 2010, 651, 27-36.	0.3	0
310	Solid-liquid interface synthesis of microcrystalline porous coordination networks. Chemical Communications, 2010, 46, 6515.	2.2	35
311	Multifunctional sensing ability of a new Pt/Zn-based luminescent coordination polymer. Dalton Transactions, 2010, 39, 3400.	1.6	45
312	Structure and dynamics of ammonium borohydride. Chemical Communications, 2010, 46, 9164.	2.2	19
313	Synthesis and crystal structure of sodium borosilicide, Na ₈ B ₇ Si _{17.5} . Dalton Transactions, 2010, 39, 10197.	1.6	13
314	Evaluation of methods to predict reactivity of gold nanoparticles. Physical Chemistry Chemical Physics, 2011, 13, 12858.	1.3	8
315	YCa ₃ (VO) ₃ (BO) ₃ : A Kagomé Compound Based on Vanadium(III) with a Highly Frustrated Ground State. Chemistry of Materials, 2011, 23, 1315-1322.	3.2	33
316	Effect of heat-treatment process on FeF ₃ nanocomposite electrodes for rechargeable Li batteries. Journal of Materials Chemistry, 2011, 21, 10035.	6.7	69
317	Controlling vanadium phosphate catalyst precursor morphology by adding alkane solvents in the reduction step of VOPO ₄ ·2H ₂ O to VOHPO ₄ ·0.5H ₂ O. Journal of Materials Chemistry, 2011, 21, 16136.	6.7	28
318	Vapour-adsorption and chromic behaviours of luminescent coordination polymers composed of a Pt(II)-diimine metalloligand and alkaline-earth metal ions. Dalton Transactions, 2011, 40, 8012.	1.6	39
319	On the growth and properties of high quality single crystals of the yttrium doped strontium cobaltates, Y _{1-x} Sr _x CoO ₃ (0.7 ≤ x ≤ 0.95). Journal of Materials Chemistry, 2011, 21, 1212-1217.	6.7	10
320	Intrinsic stoichiometry and oxygen-induced σ -type conductivity of pyrite FeS ₂ . Physical Review B, 2011, 84, .	1.1	65
321	First-Principles Calculations of Structural Changes Induced by Oxygen Vacancies in Tetragonal Phase BaTiO ₃ . Key Engineering Materials, 0, 485, 19-22.	0.4	2
322	The crystal structure of Al(OH) ₃ : Neutron diffraction measurements and ab initio calculations. American Mineralogist, 2011, 96, 854-859.	0.9	15
323	Role of alkali metal adsorption and defect position on the work function of a (5, 5) capped single-walled carbon nanotube. Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2011, 29, .	0.6	8
324	Coordination Polymers and Frameworks in Uranyl Ion Complexes with Sulfonates and Cucurbit[6]uril. Crystal Growth and Design, 2011, 11, 5702-5711.	1.4	30

#	ARTICLE	IF	CITATIONS
325	Polymorphism and phase transformations of $\text{Li}_2\text{xFeSiO}_4(0\text{a}\text{c}\frac{1}{2}\text{x}\text{a}\frac{1}{2}\text{z}2)$ from first principles. <i>Physical Review B</i> , 2011, 84, .	1.1	35
326	Antiferromagnetic superexchange via d^3 states of titanium in EuTiO_3 as seen from BaTiO_3 . <i>Physical Review B</i> , 2011, 83, .	1.1	104
327	Crystal structure and magnetic properties of IrO_2 . <i>Physical Review B</i> , 2011, 83, .	1.1	78
328	Single-side-hydrogenated graphene: Density functional theory predictions. <i>Physical Review B</i> , 2011, 84, .	1.1	80
329	Ab initio Investigations of $\text{Fe}^{2+}/\text{Fe}^{3+}$ Bond Dimerization and Ferroelectricity Induced by Intermediate Site/Bond-Centered Charge Ordering in Magnetite. <i>Journal of the Physical Society of Japan</i> , 2011, 80, 014709.	0.7	10
330	Actinide Dioxides in Water: Interactions at the Interface. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 3130-3134.	2.1	38
331	Synthesis and Crystal Structure of a Layered Silicate HUS-1 with a Halved Sodalite-Cage Topology. <i>Inorganic Chemistry</i> , 2011, 50, 2294-2301.	1.9	34
332	Structure of Ferroelectric Silver Niobate AgNbO_3 . <i>Chemistry of Materials</i> , 2011, 23, 1643-1645.	3.2	152
333	Ion-Exchange Synthesis, Crystal Structure, and Electrochemical Properties of $\text{Li}_2\text{Tl}_6\text{O}_{13}$. <i>Chemistry of Materials</i> , 2011, 23, 2344-2352.	3.2	51
334	Dramatic Structural Rearrangements in Porous Coordination Networks. <i>Journal of the American Chemical Society</i> , 2011, 133, 5853-5860.	6.6	84
335	Crystal Structure and Local Dynamics in Tetrahedral Proton-Conducting $\text{La}_{1-x}\text{Ba}_x\text{GaO}_4$. <i>Journal of Physical Chemistry C</i> , 2011, 115, 298-304.	1.5	12
336	Native Defects and the Dehydrogenation of NaBH_4 . <i>Journal of Physical Chemistry C</i> , 2011, 115, 24429-24434.	1.5	13
337	Energetics and Lateral Effects of CH_2ClF Adsorbed on Anatase TiO_2 (101) Surface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23908-23912.	1.5	2
338	Theoretical Studies on Proton Transfer among a High Density of Acid Groups: Surface of Zirconium Phosphate with Adsorbed Water Molecules. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5599-5606.	1.5	26
339	Uranyl Ion Complexation by Aliphatic Dicarboxylic Acids in the Presence of Cucurbiturils as Additional Ligands or Structure-Directing Agents. <i>Crystal Growth and Design</i> , 2011, 11, 2606-2620.	1.4	118
340	Uranyl-Alkali Metal Ion Heterometallic Complexes with Cucurbit[6]uril and a Sulfonated Catechol. <i>Crystal Growth and Design</i> , 2011, 11, 3282-3294.	1.4	62
341	Beyond Charge Density Matching: The Role of $\text{Ca}^{\text{H}}\text{O}$ Interactions in the Formation of Templated Vanadium Tellurites. <i>Crystal Growth and Design</i> , 2011, 11, 4213-4219.	1.4	16
342	Magnesium dititanate (MgTi_2O_5) with pseudobrookite structure: a review. <i>Science and Technology of Advanced Materials</i> , 2011, 12, 034301.	2.8	55

#	ARTICLE	IF	CITATIONS
343	Severe structural damage in Cr- and V-rich clinozoisite: relics of an epidote-group mineral with Ca ₂ Al ₂ Cr ₃₊ Si ₃ O ₁₂ (OH) composition?. European Journal of Mineralogy, 2011, 23, 731-743.	0.4	5
344	On the Mechanism of Carborane Diffusion on a Hydrated Silica Surface. Journal of Physical Chemistry C, 2011, 115, 108-111.	1.5	13
345	Development of a Transferable Variable Charge Potential for the Study of Energy Conversion Materials FeF ₂ and FeF ₃ . Journal of Physical Chemistry C, 2011, 115, 24198-24205.	1.5	14
346	Multi-component transparent conducting oxides: progress in materials modelling. Journal of Physics Condensed Matter, 2011, 23, 334210.	0.7	52
347	Graphene adhesion on mica: Role of surface morphology. Physical Review B, 2011, 83, .	1.1	59
348	An Approach to Control of Band Gap Energy and Photoluminescence upon Band Gap Excitation in Pr ³⁺ -Doped Perovskites La _{1/3} MO ₃ (M = Nb, Ta):Pr ³⁺ . Inorganic Chemistry, 2011, 50, 5389-5395.	1.9	42
349	A new room temperature phase of diammonium hexafluorogermanate(IV), (NH ₄) ₂ [GeF ₆]. Zeitschrift für Kristallographie, 2011, 226, .	1.1	0
350	Low-temperature phase of Li ₂ FeSiO ₄ : crystal structure and a preliminary study of electrochemical behavior. Dalton Transactions, 2011, 40, 1846.	1.6	33
351	Screening for high-performance piezoelectrics using high-throughput density functional theory. Physical Review B, 2011, 84, .	1.1	125
352	¹³ C Chemical Shifts of Propane Molecules Encaged in Structure II Clathrate Hydrate. Journal of Physical Chemistry A, 2011, 115, 643-647.	1.1	16
353	The role of intermolecular hydrogen bond on dielectric properties in hydrogen-bonded material 5-bromo-9-hydroxyphenalenone: theoretical investigation. Physical Chemistry Chemical Physics, 2011, 13, 10719.	1.3	10
354	Synthesis and Atomic Characterization of a Ti ₂ O ₃ Nanosheet. Journal of Physical Chemistry Letters, 2011, 2, 1820-1823.	2.1	25
355	Understanding the p-type defect chemistry of CuCrO ₂ . Journal of Materials Chemistry, 2011, 21, 3655.	6.7	176
356	Magnetic and diffusive nature of LiFePO ₄ investigated by muon spin rotation and relaxation. Physical Review B, 2011, 84, .	1.1	65
357	Three-Dimensional Morphology and Crystallography of Gold Nanorods. Nano Letters, 2011, 11, 273-278.	4.5	123
358	Quantum-mechanics-based design principles for solid oxide fuel cell cathode materials. Energy and Environmental Science, 2011, 4, 4933.	15.6	141
359	Spin-Wave Spectrum in a Single-Domain Magnetic Ground State of Triangular Lattice Antiferromagnet CuFeO ₂ . Journal of the Physical Society of Japan, 2011, 80, 014714.	0.7	24
360	Structure of Hydrated Sodium Ions and Water Molecules Adsorbed on the Mica/Water Interface. Journal of Physical Chemistry C, 2011, 115, 15959-15964.	1.5	41

#	ARTICLE	IF	CITATIONS
361	Presence of excited electronic state in CaWO ₄ crystals provoked by a tetrahedral distortion: An experimental and theoretical investigation. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	84
362	The structural state of lead-based relaxor ferroelectrics under pressure. <i>IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control</i> , 2011, 58, 1905-1913.	1.7	17
363	X-Ray Energy-Dispersive Spectrometry in Scanning Transmission Electron Microscopes. , 2011, , 291-351.		18
364	Modulation of the Work Function of Capped Single-Walled Carbon Nanotube by Alkali-Metal Adsorption: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8928-8933.	1.5	25
365	Fabrication and Photoluminescent Property of Transparent Nanocrystallized-Glass in Li ₂ O-ZnO-GeO ₂ System. <i>IOP Conference Series: Materials Science and Engineering</i> , 2011, 18, 112002.	0.3	0
366	Graphene/graphane interface energy and implications for defects. <i>Physical Review B</i> , 2011, 84, .	1.1	11
367	Photoluminescence Properties of BaMgAl ₁₀ O ₁₇ Doped with High Concentration of Mn ²⁺ for Blue-LED-Based Solid-State Lighting. <i>Journal of the Electrochemical Society</i> , 2011, 158, J363.	1.3	7
368	Anisotropic Thermal Properties of the Nonlinear Optical and Polar Oxide Material Na ₂ TeW ₂ O ₉ . <i>Crystal Growth and Design</i> , 2011, 11, 3636-3641.	1.4	29
369	ONDRUSITE, CaCu ₄ (AsO ₄) ₂ (AsO ₃ OH) ₂ ·10H ₂ O, A NEW MINERAL SPECIES FROM THE JACHYMOV ORE DISTRICT, CZECH REPUBLIC: DESCRIPTION AND CRYSTAL-STRUCTURE DETERMINATION. <i>Canadian Mineralogist</i> , 2011, 49, 885-897.	0.3	9
370	Synthesis, Characterization, and Structure-Property Relationships in Two New Polar Oxides: Zn ₂ (MoO ₄) ₂ (SeO ₃) and Zn ₂ (MoO ₄) ₂ (TeO ₃). <i>Inorganic Chemistry</i> , 2011, 50, 5215-5222.	1.9	73
371	Magnetic and magnetoelectric properties of Ba _{2-x} Sr _x Ni ₂ Fe ₁₂ O ₂₂ single crystals with Y-type hexaferrite structure. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	50
372	High-Pressure Synthesis and Correlation between Structure, Magnetic, and Dielectric Properties in LiNbO ₃ -Type MnMO ₃ (M = Ti, Sn). <i>Inorganic Chemistry</i> , 2011, 50, 6392-6398.	1.9	77
373	Ln ^{III} -Co-Based Rock-Salt-Type Porous Coordination Polymers: Vapor Response Controlled by Changing the Lanthanide Ion. <i>Inorganic Chemistry</i> , 2011, 50, 2061-2063.	1.9	24
374	Redetermination of synthetic warwickite, Mg ₃ TiO ₂ (BO ₃) ₂ . <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, i18-i19.	0.2	4
375	Tantalum oxide nanomesh as self-standing one nanometre thick electrolyte. <i>Energy and Environmental Science</i> , 2011, 4, 3509.	15.6	64
376	Experimental Visualization of Chemical Bonding and Structural Disorder in Hydroxyapatite through Charge and Nuclear-Density Analysis. <i>Journal of Physical Chemistry C</i> , 2011, 115, 25077-25087.	1.5	49
377	Tunable band gaps in bilayer transition-metal dichalcogenides. <i>Physical Review B</i> , 2011, 84, .	1.1	538
378	Characterization of lattice defects by x-ray absorption spectroscopy at the Zn K-edge in ferromagnetic, pure ZnO films. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	30

#	ARTICLE	IF	CITATIONS
379	First-principles calculations of lattice dynamics in CdTiO ₃ and CaTiO ₃ : Phase stability and ferroelectricity. Physical Review B, 2011, 83, .	1.1	58
380	Comparison of the defective pyrochlore and ilmenite polymorphs of AgSb ₃ O ₇ : GGA and hybrid DFT. Physical Review B, 2011, 83, .	1.1	23
381	Interfacial interactions between local defects in amorphous SiO ₂ and supported graphene. Physical Review B, 2011, 84, .	1.1	38
382	Evidence for (Bi,Pb)O Covalency in the High-T _C Ferroelectric PbTiO ₃ and BiFeO ₃ with Large Tetragonality. Chemistry of Materials, 2011, 23, 3135-3137.	3.2	102
383	Orientation relationships between icosahedral clusters in hexagonal MgZn ₂ and monoclinic Mg ₄ Zn ₇ phases in Mg-Zn(-Y) alloys. Philosophical Magazine, 2011, 91, 2634-2644.	0.7	25
384	trans-Methylpyridine cyclen versus cross-bridged trans-methylpyridine cyclen. Synthesis, acid-base and metal complexation studies (metal = Co ²⁺ , Cu ²⁺ , and Zn ²⁺). Dalton Transactions, 2011, 40, 4514.	1.6	25
385	γ-Cysteine as a Chiral Linker in Lanthanide-Cucurbit[6]uril One-Dimensional Assemblies. Inorganic Chemistry, 2011, 50, 10558-10560.	1.9	62
386	B ³⁺ hounekite, U(SO ₄) ₂ (H ₂ O) ₄ , from J ¹ chymov (St) Tj ETQq1 1 0.784314 rgBT 2011, 75, 2739-2753.	0.6	18
387	Energy barriers for trimethylaluminum reaction with varying surface hydroxyl density. Applied Surface Science, 2011, 258, 225-229.	3.1	28
388	Efficient supercell design for surface and interface calculations of hexagonal phases: Î±-Al ₂ O ₃ case study. Computational Materials Science, 2011, 50, 1197-1201.	1.4	33
389	Theoretical investigation on the transition-metal borides with Ta ₃ B ₄ -type structure: A class of hard and refractory materials. Computational Materials Science, 2011, 50, 1559-1566.	1.4	169
390	Structure and dynamics of water on Li ⁺ , Na ⁺ , K ⁺ , Cs ⁺ , H ₃ O ⁺ -exchanged muscovite surfaces: A molecular dynamics study. Geochimica Et Cosmochimica Acta, 2011, 75, 63-81.	1.6	128
391	First-principles electronic structure and relative stability of pyrite and marcasite: Implications for photovoltaic performance. Physical Review B, 2011, 83, .	1.1	122
392	Hybrid density functional study of oxygen vacancies in KTaO ₃ and NaTaO ₃ . Physical Review B, 2011, 83, .	1.1	26
393	Ab initio study of proper topological ferroelectricity in layered perovskite La ₂ Ti ₂ O ₇ . Physical Review B, 2011, 83, .	1.1	56
394	Synthesis, structure and magnetic properties of nanocrystalline YMnO ₃ . Dalton Transactions, 2011, 40, 7583.	1.6	51
395	Evaluation of Favorable-Structured Cathode Materials for Lithium-Ion Batteries Using High-Throughput Computing. Chemistry of Materials, 2011, 23, 3854-3862.	3.2	244
396	Crystal structure and X-ray diffraction data of a new hexagonal perovskite compound, Ba ₄ CuNb ₃ O ₁₂ . Powder Diffraction, 2011, 26, 244-247.	0.4	0

#	ARTICLE	IF	CITATIONS
397	Synthesis and photoluminescence of a novel Sr-SiAlON:Eu ²⁺ blue-green phosphor (Sr ₁₄ Si ₆ Al ₆ O ₁₀ :Eu ²⁺ (sâ%7)). Journal of Alloys and Compounds, 2011, 509, 332-337.	2.8	47
398	Peculiarity of component interaction in {Y, Dy}â€“Mnâ€“Sn ternary systems. Journal of Alloys and Compounds, 2011, 509, 7559-7564.	2.8	4
399	Cationic doping of MgO surfaces to build corrosion protection in Mg alloys. Journal of Alloys and Compounds, 2011, 509, 8189-8198.	2.8	25
400	Vitreous phase coating on glaserite-type alkaline earth silicate blue phosphor BaCa ₂ MgSi ₂ O ₈ :Eu ²⁺ . Journal of Alloys and Compounds, 2011, 509, 8738-8741.	2.8	15
401	Structure-Directing Roles and Interactions of Fluoride and Organocations with Siliceous Zeolite Frameworks. Journal of the American Chemical Society, 2011, 133, 18728-18741.	6.6	63
402	Investigation of hydrogen sites of wadsleyite: A neutron diffraction study. Physics of the Earth and Planetary Interiors, 2011, 189, 56-62.	0.7	28
403	First principles study on interfacial electronic structures in exchange-spring magnets. Journal of Physics: Conference Series, 2011, 266, 012046.	0.3	19
404	Theoretical Study of the Interstitial Oxygen Atom in Anatase and Rutile TiO ₂ : Electron Trapping and Elongation of the r(Oâˆ“O) Bond. Journal of Physical Chemistry C, 2011, 115, 8265-8273.	1.5	44
405	High-Pressure Synthesis, Structure, Dielectric and Magnetic Properties for SrCu ₃ Ti ₄ O ₁₂ . Ferroelectrics, 2011, 414, 180-189.	0.3	10
406	â€“Cation Polarity Control in ACuTe ₂ O ₇ (A = Sr ²⁺ ,) Tj ETQq1 1 0.784314 rgBT /Overlock 1.9 38	1.9	38
407	Analysis of lattice site occupancy in kesterite structure of Cu ₂ ZnSnS ₄ films using synchrotron radiation x-ray diffraction. Journal of Applied Physics, 2011, 110, .	1.1	65
408	Structure and dynamics of the fast lithium ion conductor â€“Li ₇ La ₃ Zr ₂ O ₁₂ â€“. Physical Chemistry Chemical Physics, 2011, 13, 19378.	1.3	559
409	Indexing, Extraction of Integrated Intensity, and Structure Solution by the Direct Method and Charge Flipping from Power X-Ray Diffraction Data. Nihon Kessho Gakkaishi, 2011, 53, 231-239.	0.0	1
410	Nucleation and Nanometric Inhomogeneity in Niobio germanate Glass: In-Situ Inelastic Light Scattering and TEM Studies. IOP Conference Series: Materials Science and Engineering, 2011, 18, 112009.	0.3	1
411	The Effect of Particle Size on Hydrogen Release from Sodium Alanate. ECS Meeting Abstracts, 2011, , .	0.0	0
412	Photoemission Study of Rh ₁₇ S ₁₅ Superconductor. Journal of the Physical Society of Japan, 2011, 80, SA111.	0.7	4
413	Relationship between Ferroelectric Property and Crystal Structure of Pb(Zr, Ti, Nb)O ₃ with High Nb Content. Funtai Oyobi Fummatsumu Yakin/Journal of the Japan Society of Powder and Powder Metallurgy, 2011, 58, 703-709.	0.1	1
414	NMR study of pyrochlore lattice antiferromagnet, melanothallite Cu ₂ OCl ₂ . Journal of Physics: Conference Series, 2011, 320, 012030.	0.3	5

#	ARTICLE	IF	CITATIONS
415	Crystal structure of layered perovskite compound, $\text{Li}_2\text{LaTa}_2\text{O}_6\text{N}$. Powder Diffraction, 2011, 26, 4-8.	0.4	12
416	Electron density distribution and crystal structure of $\text{Ca}_{1-x}/2\text{AlSi}(\text{N}_{3-x}\text{O}_x):\text{Eu}^{2+}$ ($x \approx 0.11$). Powder Diffraction, 2011, 26, S38-S43.	0.4	4
417	Rattling Vibrations Observed by Means of Single-Crystal X-ray Diffraction in the Filled Skutterudite $\text{RO}_4\text{Sb}_{12}$ ($\text{R} = \text{La}, \text{Ce}, \text{Pr}, \text{Nd}, \text{Sm}$). Journal of the Physical Society of Japan, 2011, 80, 054601.	0.7	28
418	Crystal Structure of Fast Lithium-ion-conducting Cubic $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$. Chemistry Letters, 2011, 40, 60-62.	0.7	336
419	Synthesis and Crystal Structure of Cubic Perovskite-type $\text{BaMo}_x\text{Ti}_{1-x}\text{O}_3$ with $x \approx 0.175$. Chemistry Letters, 2011, 40, 524-526.	0.7	1
420	Cation distribution analysis of Sr-La-Co M-type ferrites by neutron diffraction, extended X-ray absorption fine structure and X-ray magnetic circular dichroism. Journal of the Ceramic Society of Japan, 2011, 119, 285-290.	0.5	35
421	Magnetic Structure Determination of $\text{Ce}_2\text{Al}_{10}$ ($\text{T} = \text{Ru}$ and Os): Single Crystal Neutron Diffraction Studies. Journal of the Physical Society of Japan, 2011, 80, 073701.	0.7	68
422	Hydrogen Atom of KH_2AsO_4 Determined by Neutron Diffraction Study. Journal of the Physical Society of Japan, 2011, 80, 074607.	0.7	4
423	Gallium interstitial contributions to diffusion in gallium arsenide. AIP Advances, 2011, 1, .	0.6	8
424	Structural Study of Ordering in the Normal-Commensurate Transition of $\{\text{N}(\text{CH}_3)_4\}_2\text{MnCl}_4$ "Models and Adaptation". Journal of the Physical Society of Japan, 2011, 80, 064602.	0.7	3
425	Effect of Excess Li and Cation Mixing on Electronic Structure of $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ Cathode Active Material of Lithium-Ion Battery Investigated by First-Principle Calculation.. Electrochemistry, 2011, 79, 80-85.	0.6	2
426	Calculation of the electronic structure of delafossite AgTaN_2 from first principles. Journal of the Ceramic Society of Japan, 2011, 119, 663-666.	0.5	6
427	Investigation of the irreversible reaction mechanism and the reactive trigger on SiO anode material for lithium-ion battery. Journal of the Ceramic Society of Japan, 2011, 119, 855-860.	0.5	62
428	Dependence of Thermodynamic Stability, Crystal and Electronic Structures and Battery Characteristic on Synthetic Condition and Li Content for $\text{Li}_x\text{Mn}_{0.5}\text{Ni}_{0.5}\text{O}_2$ as a Cathode Active Material of Li-Ion Battery. Electrochemistry, 2011, 79, 15-23.	0.6	4
429	Ab initio study of $\text{Sb}_2\text{SexTe}_3$ ($x=0, 1, 2$) phase change materials. Solid State Sciences, 2011, 13, 131-134.	1.5	7
430	Mechanical properties and electronic structure of the incompressible rhenium carbides and nitrides: A first-principles study. Solid State Communications, 2011, 151, 1842-1845.	0.9	20
431	New semiconducting silicides assembled from transition-metal-encapsulating Si clusters. Thin Solid Films, 2011, 519, 8456-8460.	0.8	10
432	Prospects for lithium imaging using annular bright field scanning transmission electron microscopy: A theoretical study. Ultramicroscopy, 2011, 111, 1144-1154.	0.8	38

#	ARTICLE	IF	CITATIONS
433	The new sulphur-containing ligand 4-(4-methylthiophenyl)-3,2,6-terpyridine (L1) and the supramolecular structure of the dinuclear complex $[Zn_2(L1)_2(acac)_4]$ (acac=acetylacetonato): The key role of non-covalent C=O contacts and C-H...S hydrogen bonds. <i>Journal of Molecular Structure</i> , 2011, 1006, 684-691.	1.8	8
434	Morphology of CuO through precipitation process under 2.45GHz microwave irradiation. <i>Journal of the European Ceramic Society</i> , 2011, 31, 2441-2445.	2.8	3
435	Coupled quantum-continuum analysis of crack tip processes in aluminum. <i>Journal of the Mechanics and Physics of Solids</i> , 2011, 59, 2476-2487.	2.3	20
436	Effect of Cr and Mn ions on the structure and magnetic properties of GaFeO ₃ : Role of the substitution site. <i>Journal of Solid State Chemistry</i> , 2011, 184, 2353-2359.	1.4	16
437	Synthesis, crystal structures and photoluminescence properties of new oxyborates, Mg ₅ NbO ₃ (BO ₃) ₃ and Mg ₅ TaO ₃ (BO ₃) ₃ , with novel warwickite-type superstructures. <i>Journal of Solid State Chemistry</i> , 2011, 184, 2466-2471.	1.4	7
438	Crystal structure of Eu-doped magnetoplumbite-type lanthanum aluminum oxynitride with emission site splitting. <i>Journal of Solid State Chemistry</i> , 2011, 184, 2533-2537.	1.4	12
439	Synthesis, structure and physical properties of reduced barium titanate Ba ₂ Ti _{1.3} O ₂₂ . <i>Journal of Solid State Chemistry</i> , 2011, 184, 3117-3120.	1.4	4
440	Crystal structure of Na ₂ MMgP ₂ O ₈ (M: Ba, Sr, Ca) orthophosphates and their luminescence properties activated by Eu ²⁺ ; analogous structural behaviors of glaserite-type phosphates and silicates. <i>Journal of Solid State Chemistry</i> , 2011, 184, 3247-3252.	1.4	28
441	Electronic structure and magnetic coupling properties of EuFe ₂ P ₂ : First-principles calculations. <i>Physica B: Condensed Matter</i> , 2011, 406, 4687-4690.	1.3	5
442	The electronic structure of grain-boundary of YBa ₂ Cu ₃ O ₇ doped with 3d transition-metal atoms. <i>Physica C: Superconductivity and Its Applications</i> , 2011, 471, 1606-1615.	0.6	4
443	Preparation and crystal structure of a new bismuth vanadate, Bi _{3.33} (VO ₄) ₂ O ₂ . <i>Materials Research Bulletin</i> , 2011, 46, 962-965.	2.7	16
444	Rapid microwave synthesis of indium filled skutterudites: An energy efficient route to high performance thermoelectric materials. <i>Materials Research Bulletin</i> , 2011, 46, 2288-2290.	2.7	56
445	Influence of the exchangeable cation on the adsorption of 2-nitro-1-propanol on smectite surface models. <i>Chemical Physics Letters</i> , 2011, 515, 49-55.	1.2	3
446	Ca ²⁺ -exchanged ferrierite: Quasi one-dimensional zeolite for highly selective and stable formation of light alkenes in catalytic cracking of n-octane. <i>Applied Catalysis A: General</i> , 2011, 407, 127-133.	2.2	10
447	Molecular heterometallic hydride clusters composed of rare-earth and d-transition metals. <i>Nature Chemistry</i> , 2011, 3, 814-820.	6.6	66
448	New silica clathrate minerals that are isostructural with natural gas hydrates. <i>Nature Communications</i> , 2011, 2, 196.	5.8	120
449	Synthesis, Structural Transformation, Thermal Stability, Valence State, and Magnetic and Electronic Properties of PbNiO ₃ with Perovskite- and LiNbO ₃ -Type Structures. <i>Journal of the American Chemical Society</i> , 2011, 133, 16920-16929.	6.6	99
450	Effect of Antisite Defects on the Formation of Oxygen Vacancies in Sr ₂ FeMoO ₆ : Implications for Ion and Electron Transport. <i>Chemistry of Materials</i> , 2011, 23, 4525-4536.	3.2	108

#	ARTICLE	IF	CITATIONS
451	Monitoring the Formation of H-MCM-22 by a Combined XRPD and Computational Study of the Decomposition of the Structure Directing Agent. <i>Chemistry of Materials</i> , 2011, 23, 4900-4909.	3.2	14
452	Freezing in Resonance Structures for Better Packing: XeF_2 Becomes $(\text{XeF}^+)(\text{F}^-)$ at Large Compression. <i>Inorganic Chemistry</i> , 2011, 50, 3832-3840.	1.9	55
453	First-principles predictions of low-energy phases of multiferroic BiFeO_3 . <i>Physical Review B</i> , 2011, 83, .	1.1	216
454	Probing magnetoelastic coupling and structural changes in magnetoelectric gallium ferrite. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 445403.	0.7	45
455	Effects of Alkali Adatoms on CO and H_2S Adsorptions on the Fe(100) Surface: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23893-23901.	1.5	19
456	Ionization-Enhanced Decomposition of 2,4,6-Trinitrotoluene (TNT) Molecules. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8142-8146.	1.1	12
457	One-dimensional uranium-organic coordination polymers: crystal and electronic structures of uranyl-diacetohydroxamate. <i>Dalton Transactions</i> , 2011, 40, 6007.	1.6	17
458	Detailed Studies of a High-Capacity Electrode Material for Rechargeable Batteries, $\text{Li}_2\text{MnO}_3 \sim \text{LiCo}_{1/3}\text{Ni}_{1/3}\text{Mn}_{1/3}\text{O}_2$. <i>Journal of the American Chemical Society</i> , 2011, 133, 4404-4419.	6.6	1,066
459	Atomistic structure and energetics of interface between Mn-doped Ga_2O_3 and MgAl_2O_4 . <i>Journal of Materials Science</i> , 2011, 46, 4169-4175.	1.7	12
460	First-principles study of structure, vacancy formation, and strength of bcc Fe/V4C3 interface. <i>Journal of Materials Science</i> , 2011, 46, 4206-4215.	1.7	7
461	Effects of Mg and Si ions on the symmetry of $\gamma\text{-AlOOH}$. <i>Physics and Chemistry of Minerals</i> , 2011, 38, 727-733.	0.3	15
462	Synthesis, phase relation and electrical and electrochemical properties of ruthenium-substituted Li_2MnO_3 as a novel cathode material. <i>Journal of Power Sources</i> , 2011, 196, 6934-6938.	4.0	75
463	Preparation, crystal structure and photoluminescence of garnet-type calcium tin titanium aluminates. <i>Journal of Solid State Chemistry</i> , 2011, 184, 965-970.	1.4	7
464	Magnetic ordering of divalent europium in double perovskites $\text{Eu}_2\text{LnTaO}_6$ (Ln=rare earths). <i>Journal of Solid State Chemistry</i> , 2011, 184, 1478-1483.	1.4	7
465	Predicting metal-to-metal charge transfer in closed-shell transition metal oxides doped with Bi^{3+} or Pb^{2+} . <i>Chemical Physics Letters</i> , 2011, 503, 239-243.	1.2	69
466	High-speed epitaxial growth of (100)-oriented CeO_2 film on r-cut sapphire by laser chemical vapor deposition. <i>Surface and Coatings Technology</i> , 2011, 205, 4079-4082.	2.2	17
467	Local and Permeating Disorder of Copper(I) Cations in $\text{Cu}_3\text{Bi}_2\text{S}_2\text{Br}_2$ and $\text{Cu}_4\text{Bi}_3\text{S}_5\text{Br}_3 \cdot x\text{Cl}_x$ ($x = 1.19$). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2011, 637, 62-66.	0.6	5
468	gsaslanguage: a <i>GSAS</i> script language for automated Rietveld refinements of diffraction data. <i>Journal of Applied Crystallography</i> , 2011, 44, 873-877.	1.9	59

#	ARTICLE	IF	CITATIONS
469	Application of a theory for particle statistics to structure refinement from powder diffraction data. Journal of Applied Crystallography, 2011, 44, 921-927.	1.9	14
470	<i>VESTA</i> for three-dimensional visualization of crystal, volumetric and morphology data. Journal of Applied Crystallography, 2011, 44, 1272-1276.	1.9	16,580
471	<i>Ab initio</i> reconstruction of difference densities by charge flipping. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, 9-20.	0.3	4
472	Structures of two new high-pressure forms of AlPO_4 by X-ray powder diffraction and NMR spectroscopy. Acta Crystallographica Section B: Structural Science, 2011, 67, 30-40.	1.8	12
473	Fluorescence detection of white-beam X-ray absorption anisotropy: towards element-sensitive projections of local atomic structure. Journal of Synchrotron Radiation, 2011, 18, 851-861.	1.0	8
474	Mixed Magnetism for Refrigeration and Energy Conversion. Advanced Energy Materials, 2011, 1, 1215-1219.	10.2	227
475	Silver(II) Fluorosulfate: A Thermally Fragile Ferromagnetic Derivative of Divalent Silver in an Oxa-Ligand Environment. European Journal of Inorganic Chemistry, 2011, 2011, 2499-2507.	1.0	20
476	$\text{Ag}_3(\text{SO}_3\text{F})_4$: A Rare Example of a Mixed-Valent AgII/AgI Compound Showing 1D Antiferromagnetism. European Journal of Inorganic Chemistry, 2011, 2011, 2508-2516.	1.0	15
477	Chirality Measures for Vectors, Matrices, Operators and Functions. ChemPhysChem, 2011, 12, 197-205.	1.0	18
482	<i>Ab Initio</i> Powder Diffraction Structure Analysis of a Host-Guest Network: Short Contacts between Tetrathiafulvalene Molecules in a Pore. Angewandte Chemie - International Edition, 2011, 50, 6105-6108.	7.2	36
483	Electric Control of Magnetization and Interplay between Orbital Ordering and Ferroelectricity in a Multiferroic Metal-Organic Framework. Angewandte Chemie - International Edition, 2011, 50, 5847-5850.	7.2	249
484	Oxygen Defects and Novel Transport Mechanisms in Apatite Ionic Conductors: Combined ¹⁷ O-NMR and Modeling Studies. Angewandte Chemie - International Edition, 2011, 50, 9328-9333.	7.2	57
485	Giant Negative Thermal Expansion in the Iron Perovskite $\text{SrCu}_3\text{Fe}_4\text{O}_{12}$. Angewandte Chemie - International Edition, 2011, 50, 6579-6582.	7.2	127
486	Homogeneous Nucleophilic Radiofluorination and Fluorination with Phosphazene Hydrofluorides. Chemistry - A European Journal, 2011, 17, 7796-7805.	1.7	20
487	Crystal Structures of Ziegler-Natta Catalyst Supports. Chemistry - A European Journal, 2011, 17, 13892-13897.	1.7	24
488	Polyoxometalates containing late transition and noble metal atoms. Coordination Chemistry Reviews, 2011, 255, 1642-1685.	9.5	190
489	Structural and spectroscopic characterization of a series of potassium- and/or sodium-substituted β -tricalcium phosphate. Acta Biomaterialia, 2011, 7, 1844-1852.	4.1	63
490	Experimental and theoretical study of silicon-doped Sb_2Te_3 thin films: Structure and phase stability. Applied Surface Science, 2011, 257, 4566-4568.	3.1	18

#	ARTICLE	IF	CITATIONS
491	First-principles investigations of intermetallics in the Ca-Ge system. <i>Physica B: Condensed Matter</i> , 2011, 406, 2601-2609.	1.3	7
492	Band gap and photocatalytic properties of Ti-substituted hydroxyapatite: Comparison with anatase-TiO ₂ . <i>Journal of Molecular Catalysis A</i> , 2011, 338, 18-18.	4.8	26
493	Changes in electronic structure of Li _{2-x} CuO ₂ . <i>Journal of Power Sources</i> , 2011, 196, 6939-6942.	4.0	12
494	Crystal and electronic structure change determined by various method for delithiation process of Li _x (Ni,Mn)O ₂ -based cathode material. <i>Journal of Power Sources</i> , 2011, 196, 6651-6656.	4.0	23
495	Silver delafossite nitride, AgTaN ₂ ?. <i>Journal of Solid State Chemistry</i> , 2011, 184, 7-11.	1.4	17
496	Cu ₂₂ Bi ₁₂ S ₂₁ Cl ₁₆ A mixed conductor with fast one-dimensional copper(I) ion transport. <i>Journal of Solid State Chemistry</i> , 2011, 184, 191-198.	1.4	11
497	Magnetic properties of barium uranate Ba ₂ U ₂ O ₇ . <i>Journal of Solid State Chemistry</i> , 2011, 184, 531-535.	1.4	5
498	Structure and magnetic order in the series Bi _x RE _{1-x} Fe _{0.5} Mn _{0.5} O ₃ (RE=La,Nd). <i>Journal of Solid State Chemistry</i> , 2011, 184, 830-842.	1.4	16
499	Phase stability and chemical composition dependence of the thermoelectric properties of the type-I clathrate Ba ₈ Al _x Si _{46-x} (8 ≤ x ≤ 15). <i>Journal of Solid State Chemistry</i> , 2011, 184, 1293-1303.	1.4	67
500	Neutron diffraction study of La ₄ LiAuO ₈ : Understanding Au ³⁺ in an oxide environment. <i>Journal of Solid State Chemistry</i> , 2011, 184, 1439-1444.	1.4	7
501	Preparation of a new pyrochlore-type compound Na _{0.32} Bi _{1.68} Ti ₂ O _{6.46} (OH) _{0.44} by hydrothermal reaction. <i>Journal of Solid State Chemistry</i> , 2011, 184, 1899-1902.	1.4	15
502	Synthesis and structural characterization of Al ₇ C ₃ N ₃ -homeotypic aluminum silicon oxycarbonitride, (Al _{7-x} Si _x)(O _y C _z N _{6-y-z}) (x ^{1/4} 1.2, y ^{1/4} 1.0 and z ^{1/4} 3.5). <i>Journal of Solid State Chemistry</i> , 2011, 184, 2278-2284.	1.4	8
503	Structural, electronic and magnetic properties of negative thermal expansion material Mn ₃ Cu _{1-x} S _x N. <i>Physica B: Condensed Matter</i> , 2011, 406, 1222-1225.	1.3	2
504	Migration of adatom adsorption on graphene using DFT calculation. <i>Solid State Communications</i> , 2011, 151, 13-16.	0.9	268
505	Li-ion migration in Li ₂ FeSiO ₄ -related cathode materials: A DFT study. <i>Solid State Ionics</i> , 2011, 192, 58-64.	1.3	67
506	Surface termination of BaTiO ₃ (001) single crystals: A combined electron spectroscopic and theoretical study. <i>Surface Science</i> , 2011, 605, 158-165.	0.8	23
507	High-Temperature Thermoelectric Property of Layered La _{2-2x} Ca _{1+2x} Mn ₂ O ₇ Manganites (0.75 ≤ x ≤ 1.0). <i>Japanese Journal of Applied Physics</i> , 2011, 50, 041101.	0.8	10
508	Ab initio study of magnetoelectricity in Fe/BaTiO ₃ : the effects of n-doped perovskite interfaces. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 455902.	0.7	3

#	ARTICLE	IF	CITATIONS
509	Vacancy or not: An insight on the intrinsic vacancies in rocksalt-structured GeSbTe alloys from ab initio calculations. <i>European Physics Letters</i> , 2011, 95, 27002.	0.7	23
510	Selective adsorption of atomic hydrogen on a <i>h</i> -BN thin film. <i>Journal of Chemical Physics</i> , 2011, 135, 014706.	1.2	23
511	Preparation and Thermoelectric Properties of a Chimney-Ladder ($\text{Mn}_{1-x}\text{Fe}_x\text{Si}^{\uparrow 3}$) ($\text{I}^{\uparrow 3}\text{a}^{\uparrow 1/4}$ 1.7) Solid Solution. <i>Japanese Journal of Applied Physics</i> , 2011, 50, 035804.	0.8	30
512	Ab initio study of the intrinsic exchange bias at the $\text{SrRuO}_3/\text{SrMnO}_3$ interface. <i>Physical Review B</i> , 2011, 84, 040408.	1.1	23
513	Dynamics of photoinduced phenomena in $\text{Ba}_2\text{Cu}_3\text{As}_2\text{O}_{10}$. <i>Physical Review B</i> , 2011, 84, 040408.	1.1	4
514	Ferroelectric charge ordering in LuFeO_3 and its relation to magnetic order. <i>Physical Review B</i> , 2011, 84, 040408.	1.1	26
515	Electrical and magnetic properties of the complete solid solution series between SrRuO_3 and LaRhO_3 : Filling g_2 versus tilting. <i>Physical Review B</i> , 2011, 83, .	1.1	21
516	Spin fluctuations and unconventional pairing in KFeAs . <i>Physical Review B</i> , 2011, 84, .	1.1	52
517	Competition between vanadium tetramerization and trimerization in $\text{Ba}_2\text{Cu}_3\text{As}_2\text{O}_{10}$. <i>Physical Review B</i> , 2011, 84, .	1.1	16
518	Crystal field splitting and orbital ordering in Sr_2VO_4 . <i>Physical Review B</i> , 2011, 84, .	1.1	7
519	The covalent bonding interaction in the ferroelectric LuMnO_3 . <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	7
520	Magnons and electromagnons in a spin-lattice-coupled frustrated magnet CuFeO_2 as seen via inelastic neutron scattering. <i>Physical Review B</i> , 2011, 84, .	1.1	37
521	Magnetodielectric response of square-coordinated MnO_2 unit in cubic $\text{BiMn}_7\text{O}_{12}$. <i>Applied Physics Letters</i> , 2011, 98, 072903.	1.5	9
522	Integer spin chain and nonmagnetism of the CaRuO_3 oxide. <i>Physical Review B</i> , 2011, 84, .	1.1	24
523	Electronic structure, Born effective charges and spontaneous polarization in magnetoelectric gallium ferrite. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 325902.	0.7	39
524	Magnetic order of the hexagonal rare-earth manganite YMnO_3 . <i>Physical Review B</i> , 2011, 84, .	1.1	12
525	Formation and diffusion of vacancy-polaron complex in olivine-type LiMnPO_4 and LiFePO_4 . <i>Physical Review B</i> , 2011, 84, .	1.1	40
526	Polarity replication across <i>m</i> -plane GaN/ZnO interfaces. <i>Applied Physics Letters</i> , 2011, 99, 181910.	1.5	4

#	ARTICLE	IF	CITATIONS
527	Surface ferromagnetism in hydrogenated-ZnO film. Applied Physics Letters, 2011, 98, .	1.5	42
528	Quasi-one-dimensional electronic structure of hollandite ruthenate K_2RuO_6 and high-temperature interlayer magnetoresistance in La_2O_3 doped K_2RuO_6 . Physical Review B, 2011, 84, .	1.1	16
529	High-temperature interlayer magnetoresistance in La_2O_3 doped K_2RuO_6 . Physical Review B, 2011, 84, .	1.1	4
530	Successive magnetic transitions and static magnetic order in $RCoAsO$ ($R=La, Ce, Pr, Nd, Sm, Gd$) confirmed by muon-spin rotation and relaxation. Physical Review B, 2011, 84, .	1.1	12
531	<i>Ab initio</i> study of pressure stabilized NiTi allotropes: Pressure-induced transformations and hysteresis loops. Physical Review B, 2011, 84, .	1.1	34
532	Stability of spontaneous polarization in ultrathin improper ferroelectrics. Physical Review B, 2011, 84, .	1.1	3
533	<i>Ab initio</i> structure prediction for lead sulfide at standard and elevated pressures. Physical Review B, 2011, 84, .	1.1	71
534	Orbital-separation approach for consideration of finite electric bias within density-functional total-energy formalism. Physical Review B, 2011, 84, .	1.1	11
535	Non-one-dimensional behavior in charge-ordered structurally quasi-one-dimensional $SrCo_6O_{13}$. Physical Review B, 2011, 84, .	1.1	49
536	Structural and electronic properties of Y_2O_3 of yttrium above 206 GPa from first principles. Physical Review B, 2011, 84, .	1.1	11
537	Ternary silicon germanium nitrides: A class of tunable band gap materials. Physical Review B, 2011, 84, .	1.1	11
538	First-principles structural optimization and electronic structure of the superconductor picene for various potassium doping levels. Physical Review B, 2011, 84, .	1.1	54
539	Mechanism of ferroelectric instabilities in non- AB_2O_4 type $LaCrO_3$. Physical Review B, 2011, 84, .	1.1	31
540	Stabilizing Graphitic Thin Films of Wurtzite Materials by Epitaxial Strain. Physical Review Letters, 2011, 107, 236101.	2.9	88
541	Synthesis and properties of platinum hydride. Physical Review B, 2011, 83, .	1.1	75
542	Role of interfacial transition layers in VO_2/Al_2O_3 heterostructures. Journal of Applied Physics, 2011, 110, .	1.1	66
543	<i>Ab initio</i> and atomistic study of ferroelectricity in copper-doped potassium niobate. Physical Review B, 2011, 84, .	1.1	12
544	A design of backing seat and gasket assembly in diamond anvil cell for accurate single crystal x-ray diffraction to 5 GPa. Review of Scientific Instruments, 2011, 82, 105107.	0.6	12

#	ARTICLE	IF	CITATIONS
545	Half-metallic ferrimagnetism driven by Coulomb-enhanced spin-orbit coupling in PdCrO $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$. Physical Review B, 2011, 84, .	1.1	13
546	Three-dimensional visualization of electron- and nuclear-density distributions in inorganic materials by MEM-based technology. IOP Conference Series: Materials Science and Engineering, 2011, 18, 022001.	0.3	46
547	Electronic and thermoelectric analysis of phases in the In ₂ O ₃ (ZnO) _k system. Journal of Applied Physics, 2011, 109, .	1.1	36
548	Crystal Structure Analysis of Layered Compounds Co _x TiS ₂ . Journal of the Physical Society of Japan, 2011, 80, 044601.	0.7	8
549	Crystallization and Morphology of Glassy Sanbornite. Key Engineering Materials, 0, 485, 301-304.	0.4	7
550	Synthesis and Electron Density Analysis of SnO ₂ Nano Particles. Materials Science Forum, 2011, 671, 121-129.	0.3	0
551	Effect of Sn and Nb on generalized stacking fault energy surfaces in zirconium and gamma hydride habit planes. Philosophical Magazine, 2011, 91, 1665-1678.	0.7	20
552	A Theoretical Estimation of the Charge Density Distribution in the Diluted Magnetic Semiconductors of Si _{1-x} M _x and Ge _{1-x} M _x (M = V, Mn, Co). Materials Science Forum, 2011, 699, 167-183.	0.3	0
553	Characterization of Carbon Composite LiMn _{1-x} FexPO ₄ Cathodes. IOP Conference Series: Materials Science and Engineering, 2011, 18, 122002.	0.3	3
554	Fetuin-A Regulation of Calcified Matrix Metabolism. Circulation Research, 2011, 108, 1494-1509.	2.0	322
555	X-Ray Studies on PbS. Materials Science Forum, 0, 699, 153-165.	0.3	0
556	La ₅ Zn ₂ Sn. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, i65-i65.	0.2	7
557	The modulation and reconstruction of a BiO layer of cuprate Bi ₂ 212. Superconductor Science and Technology, 2011, 24, 105007.	1.8	5
558	Dipotassium hexaaquanickel(II) bis[hexafluoridozirconate(IV)]. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, i6-i7.	0.2	4
559	LaZn _{12.37} , a zinc-deficient variant of the NaZn ₁₃ structure type. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, i43-i43.	0.2	6
560	rac-8a'-Methyl-3,4,8a'-tetrahydro-2H-spiro[[1,3]dioxolane-2,1-naphthalen]-6(7H)-one. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2460-o2460.	0.2	3
561	Relationship between oxide-ion conductivity and ordering of oxygen vacancy in the Ln ₂ Zr ₂ O ₇ (Ln= La, Tj) ETQq0 0 0 rgBT /Overlock 10 T Engineering, 2011, 18, 132003.	0.3	14
562	Piezoelectric Properties of (Li, Na, K)NbO ₃ Ceramics with Monoclinic System. Key Engineering Materials, 2011, 485, 57-60.	0.4	8

#	ARTICLE	IF	CITATIONS
563	Phase Relation of Fe ₂ -VS ₂ System and New Phase of Defect Troilite Structure. Solid State Phenomena, 0, 170, 92-96.	0.3	1
564	Superconductivity in W ₅ SiB ₂ with the T ₂ Phase Structure. Journal of the Physical Society of Japan, 2011, 80, 024702.	0.7	19
565	Relationship Between Oxide-Ion Conductivity and Ordering of Oxygen Vacancy in the Ln ₂ Zr ₂ O ₇ (Ln = La, Tj ETQq 0 0 0 rgBT / 0.8 18	0.8	18
566	Atomic-scale insight and design principles for turbine engine thermal barrier coatings from theory. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 5480-5487.	3.3	37
567	Crystal chemistry of Ti-rich ferriallanite-(Ce) from Cape Ashizuri, Shikoku Island, Japan. American Mineralogist, 2011, 96, 1870-1877.	0.9	7
568	Antimony desinsertion reaction from Sb _x CoSb _{3-<i>x</i>} . Journal of Applied Physics, 2011, 110, 043529.	1.1	5
569	<i>Ab-initio</i> approach to the electronic, structural, elastic, and finite-temperature thermodynamic properties of Ti ₂ AX (A = Al or Ga and X = C or N). Journal of Applied Physics, 2011, 110, .	1.1	35
570	The Bonding Electron Density in Aluminum. Science, 2011, 331, 1583-1586.	6.0	141
571	Theoretical studies on clean and adsorbed surfaces of Ag-In-Yb. Philosophical Magazine, 2011, 91, 2913-2919.	0.7	4
572	Structural Reinvestigation of Alkali Hexatitanate. Solid State Phenomena, 2011, 170, 208-212.	0.3	0
573	Plimerite from Krásko near Horná Slavkov ore district, Czech Republic. Journal of Geosciences (Czech) Tj ETQq 0 0 0 rgBT / Overlock 10 T 0.8 7	0.8	7
574	C ₆₀ -mediated hydrogen desorption in Li-N-H systems. Nanotechnology, 2012, 23, 485406.	1.3	5
575	Effect of C doping on the structural and electronic properties of LiFePO ₄ : A first-principles investigation. Chinese Physics B, 2012, 21, 097401.	0.7	10
576	Elastic properties of Nb-based alloys by using the density functional theory. Chinese Physics B, 2012, 21, 016202.	0.7	17
577	Superconductivity in Novel BiS ₂ -Based Layered Superconductor LaO _{1-x} F _x BiS ₂ . Journal of the Physical Society of Japan, 2012, 81, 114725.	0.7	397
578	High-temperature synchrotron X-ray powder diffraction study of Cs ₂ XSi ₅ O ₁₂ (X = Cd, Cu, Zn) leucites. Mineralogical Magazine, 2012, 76, 1257-1280.	0.6	9
579	A First-Principles Study of the Ferroelectric Phase of AgNbO ₃ . Japanese Journal of Applied Physics, 2012, 51, 09LE02.	0.8	8
580	Diffusion and segregation of niobium in fcc-nickel. Journal of Physics Condensed Matter, 2012, 24, 095010.	0.7	15

#	Magnetic interactions in the multiferroic phase of CuFe	IF	CITATIONS
581	Observation of persistent centrosymmetry in the hexagonal manganite family. Physical Review B, 2012, 85, .	1.1	17
582	Nazca Lines by La ordering in La _{2/3} xLi ₃ TiO ₃ ion-conductive perovskite. Applied Physics Letters, 2012, 101, 073903.	1.5	8
584	Change of phonon Raman spectra with V trimerization in BaV	1.1	4
585	Local structural motifs and extended-range order in liquid and solid ammonia under pressure. Physical Review B, 2012, 85, .	1.1	12
586	Disordered stoichiometric nanorods and ordered off-stoichiometric nanoparticles in n-type thermoelectric Bi ₂ Te _{2.7} Se _{0.3} . Journal of Applied Physics, 2012, 112, 093518.	1.1	5
587	Ab initio determination of crystal structures of the thermoelectric material MgAgSb. Physical Review B, 2012, 85, .	1.1	86
588	Response of the Shockley surface state to an external electrical field: A density-functional theory study of Cu(111). Physical Review B, 2012, 85, .	1.1	43
589	Mixed-valence-driven heavy-fermion behavior and superconductivity in KNi	1.1	19
590	Improvement of Stability at Low Potential and Structure of Cobalt Oxyhydroxide/CeO ₂ Composite as Additive for Nickel Hydroxide Electrode. Journal of the Electrochemical Society, 2012, 159, A2069-A2075.	1.1	71
591	Ductilizing Bulk Metallic Glass Composite by Tailoring Stacking Fault Energy. Physical Review Letters, 2012, 109, 245506.	1.3	2
592	Study on ferromagnetic hollandite K	2.9	85
593	Magnetic and structural phase diagram of Cr	1.1	25
594	Ab initio study of the factors affecting the ground state of rare-earth nickelates. Physical Review B, 2012, 85, .	1.1	23
595	CuI interlayers in lead phthalocyanine thin films enhance near-infrared light absorption. Applied Physics Letters, 2012, 100, 263303.	1.1	18
596	Ab initio two-dimensional multiband low-energy models of EtMe	1.5	27
597	Ab initio study of the factors affecting the ground state of rare-earth nickelates. Physical Review B, 2012, 85, .	1.1	56
598	Ab initio study of the factors affecting the ground state of rare-earth nickelates. Physical Review B, 2012, 85, .	1.1	4

#	ARTICLE	IF	CITATIONS
599	Stability of Ge on Si (1 1 10) surfaces and the role of dimer tilting. <i>Physical Review B</i> , 2012, 85, .	1.1	25
600	First-principles calculation of x-ray absorption spectra and x-ray magnetic circular dichroism of ultrathin Fe films on BaTiO ₃ (001). <i>Physical Review B</i> , 2012, 85, .	1.1	16
601	Structural and magnetic characterization of the complete delafossite solid solution (CuAlO ₂) _{1-x} (CuCrO ₂) _x . <i>Journal of Physics Condensed Matter</i> , 2012, 24, 016002.	0.7	5
602	The kinetics of clustering in Al-Mg-Si alloys studied by Monte Carlo simulation. <i>International Journal of Materials Research</i> , 2012, 103, 980-986.	0.1	18
603	Cage occupancies in the high pressure structure H methane hydrate: A neutron diffraction study. <i>Journal of Chemical Physics</i> , 2012, 136, 054502.	1.2	29
604	Sol-Gel Synthesis of Single Phase, High Quantum Efficiency LiCaPO ₄ :Eu ²⁺ Phosphors. <i>ECS Journal of Solid State Science and Technology</i> , 2012, 1, R37-R40.	0.9	23
605	Crystal Structure and Phase Transition Behavior of Dioctadecyldimethylammonium Chloride Monohydrate. <i>Molecular Crystals and Liquid Crystals</i> , 2012, 563, 58-66.	0.4	6
606	Charge and orbital order in frustrated Pb ₃ Mn ₇ O ₁₅ . <i>Journal of Physics Condensed Matter</i> , 2012, 24, 186002.	0.7	6
607	Redetermination of LaZn ₅ based on single crystal X-ray diffraction data. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012, 68, i1-i1.	0.2	7
608	1-(2,2-Diphenylethyl)-1H-tetrazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012, 68, o2231-o2231.	0.2	0
609	Enhanced Thermoelectric Performance of a Chimney-Ladder (Mn _{1-x} Cr _x)Si ₃ (x=1.7) Solid Solution. <i>Japanese Journal of Applied Physics</i> , 2012, 51, 085801.	0.8	42
610	Oxygen Partial Pressure Dependence of In Situ X-Ray Absorption Spectroscopy at Co and Fe K-Edge for (La _{0.6} Sr _{0.4})(Co _{0.2} Fe _{0.8})O ₃ . <i>Journal of Fuel Cell Science and Technology</i> , 2012, 9, .	0.8	2
611	Lattice-Defect Control for High-Performance Bismuth-Based Ferroelectric/Piezoelectric Crystals. <i>Funtai Oyobi Fumatsu Yakin/Journal of the Japan Society of Powder and Powder Metallurgy</i> , 2012, 59, 22-28.	0.1	0
612	Physical properties of the novel layered cobalt oxyphosphide Sr ₂ ScCoPO ₃ . <i>Journal of Physics: Conference Series</i> , 2012, 400, 022091.	0.3	5
613	Hollandite ruthenate K ₂ Ru ₈ O ₁₆ as a new Tomonaga-Luttinger-liquid system. <i>Journal of Physics: Conference Series</i> , 2012, 400, 042063.	0.3	1
614	Magnetic Excitation in Totally Symmetric Staggered Ordered Phase of PrFe ₄ P ₁₂ . <i>Journal of the Physical Society of Japan</i> , 2012, 81, 094711.	0.7	12
615	Crystal Structures and Electrode Performance of Alpha-NaFeO ₂ for Rechargeable Sodium Batteries. <i>Electrochemistry</i> , 2012, 80, 716-719.	0.6	329
616	Effect of Al-doping on crystal structure and ionic conductivity of apatite-type La _{9.33+x} /3Si _{6-x} Al _x O ₂₆ solid electrolytes. <i>Journal of the Ceramic Society of Japan</i> , 2012, 120, 74-76.	0.5	4

#	ARTICLE	IF	CITATIONS
617	A Comparison of Crystal Structures and Electrode Performance between Na ₂ FePO ₄ F and Na ₂ Fe _{0.5} Mn _{0.5} PO ₄ F Synthesized by Solid-State Method for Rechargeable Na-Ion Batteries. <i>Electrochemistry</i> , 2012, 80, 80-84.	0.6	72
618	Effect of Serine and Arginine on the Phase Transition from Amorphous CaCO ₃ and CaCO ₃ ·6H ₂ O to Calcite Film. <i>Materials Transactions</i> , 2012, 53, 1732-1738.	0.4	6
619	Density functional investigations on electronic structures, magnetic ordering and ferroelectric phase transition in multiferroic Bi ₂ NiMnO ₆ . <i>AIP Advances</i> , 2012, 2, .	0.6	14
620	Anomalous electronic structures of transition-metal oxides with hollandite-type crystal structure. <i>Journal of Physics: Conference Series</i> , 2012, 391, 012109.	0.3	2
621	Milling-induced polymorphic transformation in MoSi ₂ . <i>International Journal of Materials Research</i> , 2012, 103, 1130-1136.	0.1	2
622	Comparative Study of Absorption Spectra of V ²⁺ , Cr ³⁺ , and Mn ⁴⁺ in LaAlO_3 Based on First-Principles Configuration Interaction Calculations. <i>Journal of the Physical Society of Japan</i> , 2012, 81, 104709.	0.7	29
623	Orientation Relationships between Precipitates and Their Parent Phases in Steels at Low Transformation Temperatures. <i>Journal of Solid Mechanics and Materials Engineering</i> , 2012, 6, 323-338.	0.5	8
624	Strained and Unstrained Macrocycles Composed of Carbazole and Butadiyne Units: Electronic State and Optical Properties. <i>Journal of Organic Chemistry</i> , 2012, 77, 4837-4841.	1.7	10
625	RECENT PROGRESS OF MULTIFERROIC PEROVSKITE MANGANITES. <i>Modern Physics Letters B</i> , 2012, 26, 1230004.	1.0	114
626	Crystal and Electronic Structure Analyses on Bi ₂ SiO ₅ Added SrBi ₂ (Ta _{1-x} Nb _x) ₂ O ₉ by Using Pulsed Neutron and Synchrotron X-Ray Sources. <i>Journal of the American Ceramic Society</i> , 2012, 95, 3906-3911.	1.9	6
627	Crystal and Electronic Structure and Magnetic Properties of Divalent Europium Perovskite Oxides Eu _M O ₃ (<i>M</i> = Ti, Zr, and Hf): Experimental and First-Principles Approaches. <i>Inorganic Chemistry</i> , 2012, 51, 4560-4567.	1.9	54
628	Ab Initio Study of the Sodium Intercalation and Intermediate Phases in Na _{0.44} MnO ₂ for Sodium-Ion Battery. <i>Chemistry of Materials</i> , 2012, 24, 1205-1211.	3.2	223
629	Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives. <i>Journal of the American Chemical Society</i> , 2012, 134, 17221-17233.	6.6	182
630	Low-energy structures of zinc borohydride Zn(BH ₄) ₂ . <i>Physical Review B</i> , 2012, 86, .	1.1	27
631	Controllable chirality-induced geometrical Hall effect in a frustrated highly correlated metal. <i>Nature Communications</i> , 2012, 3, 1067.	5.8	51
632	Layered Hydride CaNiGeH with a ZrCuSiAs-type Structure: Crystal Structure, Chemical Bonding, and Magnetism Induced by Mn Doping. <i>Journal of the American Chemical Society</i> , 2012, 134, 11687-11694.	6.6	19
633	Electron paramagnetic resonance parameters for Co ²⁺ -doped in ZnO. <i>Physica Scripta</i> , 2012, T149, 014058.	1.2	3
634	Exceptionally large room-temperature ferroelectric polarization in the PbNiO ₃ multiferroic nickelate: First-principles study. <i>Physical Review B</i> , 2012, 86, .	1.1	36

#	ARTICLE	IF	CITATIONS
635	Comparative Study of Multiplet Structures of Mn^{4+} in K_2SiF_6 , K_2GeF_6 , and K_2TiF_6 Based on First-Principles Configuration Interaction Calculations. Japanese Journal of Applied Physics, 2012, 51, 022604.	0.8	38
637	High Voltage Pyrophosphate Cathode: Insights into Local Structure and Lithium Diffusion Pathways. Angewandte Chemie - International Edition, 2012, 51, 13149-13153.	7.2	74
638	Structure and nuclear density distribution in the cheralite $CaTh(PO_4)_2$: studies of its behaviour under high pressure (36 GPa). Physics and Chemistry of Minerals, 2012, 39, 685-692.	0.3	12
639	Electron trapping at the lattice Ti atoms adjacent to the Nb dopant in Nb-doped rutile TiO_2 . Journal of Materials Science, 2012, 47, 7522-7529.	1.7	9
640	A photoactive titanate with a stereochemically active Sn lone pair: Electronic and crystal structure of Sn_2TiO_4 from computational chemistry. Journal of Solid State Chemistry, 2012, 196, 157-160.	1.4	24
641	Syntheses, crystal structures, and characterization of two new $Tl^{+}Cu_2^{+}Te_6^{+}$ oxides: Tl_4CuTeO_6 and $Tl_6CuTe_2O_{10}$. Journal of Solid State Chemistry, 2012, 196, 607-613.	1.4	7
642	Experimental charge density of hematite in its magnetic low temperature and high temperature phases. Ultramicroscopy, 2012, 120, 1-9.	0.8	6
643	Screened hybrid functional applied to d^3 transition metal oxides. Diffusive behavior in $Li_xMn_2O_4$. d^3	1.1	146
644	Diffusive behavior in $Li_xMn_2O_4$. MPO_{4-n} transition-metal oxides with Mn^{4+} .	1.1	51
645	First-Principles Electronic Structure of Superconductor $Ca_4Al_2O_6Fe_2P_2$: Comparison with $LaFePO_4$ and $Ca_4Al_2O_6Fe_2As_2$. Journal of the Physical Society of Japan, 2012, 81, 014701.	0.7	5
646	Electron localization morphology of the stacking faults in Mg: A first-principles study. Chemical Physics Letters, 2012, 551, 121-125.	1.2	37
647	Crystal structure of $CaRhO_3$ polymorph: High-pressure intermediate phase between perovskite and post-perovskite. American Mineralogist, 2012, 97, 159-163.	0.9	12
648	Amorphization and amorphous stability of Bi_2Te_3 chalcogenide films. Applied Physics Letters, 2012, 100, .	1.5	10
649	Crystal and electronic structure, lattice dynamics and thermal properties of $Ag(i)(SO_3)R$ ($R = F, CF_3$) Lewis acids in the solid state. Dalton Transactions, 2012, 41, 2034-2047.	1.6	28
650	Role of Hydrogen-Bonding in the Formation of Polar Achiral and Nonpolar Chiral Vanadium Selenite Frameworks. Inorganic Chemistry, 2012, 51, 11040-11048.	1.9	25
651	Stability of Gas-Phase Tartaric Acid Anions Investigated by Quantum Chemistry, Mass Spectrometry, and Infrared Spectroscopy. Journal of Physical Chemistry A, 2012, 116, 4789-4800.	1.1	7
652	Full structural and electrochemical characterization of $Li_2Ti_6O_{13}$ as anode for Li-ion batteries. Physical Chemistry Chemical Physics, 2012, 14, 2892.	1.3	24
653	Structural phase transitions induced by pressure in ammonium borohydride. Physical Chemistry Chemical Physics, 2012, 14, 7005.	1.3	6

#	ARTICLE	IF	CITATIONS
654	The first-principles treatment of the electron-correlation and spin-orbital effects in uranium mononitride nuclear fuels. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4482.	1.3	70
655	First-principles density functional calculation of electrochemical stability of fast Li ion conducting garnet-type oxides. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10008.	1.3	66
656	Uranyl-lanthanide heterometallic assemblies with 1,2-ethanedisulfonate and cucurbit[6]uril ligands. <i>CrystEngComm</i> , 2012, 14, 3363.	1.3	40
657	Fabrication and photocatalytic performance of highly crystalline nanosheets derived from flux-grown KNb_3O_8 crystals. <i>CrystEngComm</i> , 2012, 14, 987-992.	1.3	27
658	Uranyl and mixed uranyl-lanthanide complexes with p-sulfonatocalix[4]arene. <i>CrystEngComm</i> , 2012, 14, 6369.	1.3	27
659	Electrochemical and Thermal Properties of NASICON Structured $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ as a Sodium Rechargeable Battery Cathode: A Combined Experimental and Theoretical Study. <i>Journal of the Electrochemical Society</i> , 2012, 159, A1393-A1397.	1.3	316
660	Atomic-scale structure and band-gap bowing in $\text{Cu}(\text{In,Ga})\text{Se}$. <i>Physical Review B</i> , 2012, 85, .	1.1	36
661	Anisotropic elasticity of DyScO_3 substrates. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 385404.	0.7	16
662	Ab initio derivation of electronic low-energy models for C_{60} and aromatic compounds. <i>Physical Review B</i> , 2012, 85, .	1.1	83
663	High-pressure and high-temperature phase transitions in FeTiO_3 and a new dense FeTi_3O_7 structure. <i>American Mineralogist</i> , 2012, 97, 568-572.	0.9	45
664	Soluble Zintl Phases $\text{A}_{14}\text{ZnGe}_{16}$ ($\text{A} = \text{K, Rb}$) Featuring $[\text{I}^3\text{-Ge}_4\text{Zn}(\text{I}^2\text{-Ge}_4)]^{6-}$ and $[\text{Ge}_4]^{4-}$ Clusters and the Isolation of $[(\text{MesCu})_2(\text{I}^3, \text{I}^3\text{-Ge}_4)]^{4-}$: The Missing Link in the Solution Chemistry of Tetrahedral Group 14 Element Zintl Clusters. <i>Journal of the American Chemical Society</i> , 2012, 134, 14450-14460.	6.6	47
665	Lanthanide Ion Complexes with 2-, 3-, or 4-Sulfobenzoate and Cucurbit[6]uril. <i>Crystal Growth and Design</i> , 2012, 12, 1632-1640.	1.4	40
666	Synthesis, Structure, and Characterization of New Li-Lone-Pair Oxides: Noncentrosymmetric Polar $\text{Li}_6(\text{Mo}_2\text{O}_5)_3(\text{SeO}_3)_6$ and Centrosymmetric $\text{Li}_2(\text{MO}_3)(\text{TeO}_3)$ ($\text{M} = \text{Mo}^{6+}$ or W^{6+}). <i>Inorganic Chemistry</i> , 2012, 51, 9529-9538.	1.9	44
667	The Influence of Surface Structure on H_4SiO_4 Oligomerization on Rutile and Amorphous TiO_2 Surfaces: An ATR-IR and Synchrotron XPS Study. <i>Langmuir</i> , 2012, 28, 16890-16899.	1.6	16
668	Kinetics of Anatase Electrodes: The Role of Ordering, Anisotropy, and Shape Memory Effects. <i>Chemistry of Materials</i> , 2012, 24, 2894-2898.	3.2	90
669	First-principles study of lithium ion migration in lithium transition metal oxides with spinel structure. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13963.	1.3	64
670	Solvothermal Synthesis of β -LIT-type Zeolite. <i>Crystal Growth and Design</i> , 2012, 12, 1752-1761.	1.4	24
671	Structural Analysis during Charge-Discharge Process of $\text{Li}_2\text{FeSiO}_4$ Synthesized by Molten Carbonate Flux Method. <i>Journal of the Electrochemical Society</i> , 2012, 159, A525-A531.	1.3	19

#	ARTICLE	IF	CITATIONS
672	Strain-Induced ZnO Spinterfaces. Journal of Physical Chemistry C, 2012, 116, 610-617.	1.5	14
673	Uranyl Ion Complexes with Ammoniobenzoates as Assemblers for Cucurbit[6]uril Molecules. Crystal Growth and Design, 2012, 12, 499-507.	1.4	48
674	Maximally localized Wannier functions in LaMnO ₃ within PBE + <i>U</i> , hybrid functionals and partially self-consistent GW: an efficient route to construct <i>ab initio</i> tight-binding parameters for <i>eg</i> perovskites. Journal of Physics Condensed Matter, 2012, 24, 235602.	0.7	106
675	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$ -based layered superconductor Bi ₂ O ₄ . http://www.w3.org/1998/Math/MathML	1.1	373
676	Synthesis of Heterocoordinated Atom-Containing Zeotypes Utilizing a Mechanochemical Reaction. Crystal Growth and Design, 2012, 12, 1354-1361.	1.4	12
677	Distinct ²⁹ Si MAS NMR Peaks from Si-Al Permutation on Neighboring T Sites of Unequal Si-O-T Angles: Direct Evidence from <i>J</i> -Resolved Experiment on K-Cymrite (KAlSi ₃ O ₈ ·H ₂ O). Journal of Physical Chemistry C, 2012, 116, 10714-10722.	1.5	7
678	Ferromagnetic Hollandite K ₂ Cr ₈ O ₁₆ . Physics Procedia, 2012, 30, 186-189.	1.2	3
679	Magnetic and Diffusive Nature of LiFePO ₄ . Physics Procedia, 2012, 30, 190-193.	1.2	4
680	Understanding the chiral selectivity of gold nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 2707-2711.	0.9	6
681	Passivation effect of allylamine molecule on the electronic structure of a Si(001) $\sqrt{2 \times 2}$ surface. Surface Science, 2012, 606, 470-474.	0.8	3
682	Effect of nitrogen incorporation and oxygen vacancy on electronic structure and the absence of a gap state in HfSiO films. Surface Science, 2012, 606, L64-L68.	0.8	4
683	Symmetry-Driven Novel Kondo Effect in a Molecule. Physical Review Letters, 2012, 109, 086602.	2.9	138
684	Series of Mixed Uranyl-Lanthanide (Ce, Nd) Organic Coordination Polymers with Aromatic Polycarboxylates Linkers. Inorganic Chemistry, 2012, 51, 9610-9618.	1.9	84
685	A Computational Investigation of Li ₉ M ₃ (P ₂ O ₇) ₃ (PO ₄) ₂ (M) Tj ETQ ₁ 1 0.784	1.1	17
686	Site-selective quantum correlations revealed by magnetic anisotropy in the tetramer system SeCuO ₃ . Physical Review B, 2012, 86, .	1.1	17
687	Energy Landscape Investigations Using the Prescribed Path Method in the ZnO System. Journal of Physical Chemistry C, 2012, 116, 16726-16739.	1.5	34
688	First Principles Simulations of the Electrochemical Lithiation and Delithiation of Faceted Crystalline Silicon. Journal of the American Chemical Society, 2012, 134, 14362-14374.	6.6	221
689	<i>ab initio</i> prediction of environmental embrittlement at a crack tip in aluminum. Physical Review B, 2012, 86, .	1.1	34

#	ARTICLE	IF	CITATIONS
690	Investigations of new barium dicarboxylates. Zeitschrift Fur Kristallographie - Crystalline Materials, 2012, 227, 629-634.	0.4	7
691	Systematic structural control of multichromic platinum(Pt^{II})-diimine complexes ranging from ionic solid to coordination polymer. Dalton Transactions, 2012, 41, 1878-1888.	1.6	22
692	Palenzonaite, berzeliite, and manganberzeliite: $(\text{As}^{\text{V}}, \text{V}^{\text{V}})$ Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (Stk 1081-1097.	0.6	9
693	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. Journal of Physical Chemistry C, 2012, 116, 9221-9226.	1.5	78
694	Tuning of CeO ₂ buffer layers for coated superconductors through doping. Applied Surface Science, 2012, 260, 32-35.	3.1	29
695	Adsorption and surface reaction of bis-diethylaminosilane as a Si precursor on an OH-terminated Si (0) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 667 Td (Stk 27	3.1	27
696	High-speed epitaxial growth of BaTi ₂ O ₅ thick films and their in-plane orientations. Applied Surface Science, 2012, 259, 178-185.	3.1	20
697	Sr ₇ Ge ₆ , Ba ₇ Ge ₆ and Ba ₃ Sn ₂ – Three new binary compounds containing dumbbells and four-membered chains of tetrel atoms with considerable Ge–Ge π -bonding character. Journal of Solid State Chemistry, 2012, 191, 76-89.	1.4	18
698	SrZn ₂ Sn ₂ and Ca ₂ Zn ₃ Sn ₆ – two new Ae–Zn–Sn polar intermetallic compounds (Ae: alkaline earth) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 Td (Stk 5	1.4	5
699	Synthesis and spectroscopic characterization of YPO ₄ activated with Tb ³⁺ and effect of Bi ³⁺ co-doping on the luminescence properties. Journal of Solid State Chemistry, 2012, 192, 289-295.	1.4	24
700	First-principles investigation of mechanical and thermodynamic properties of the rare earth intermetallic YbAl ₃ under pressure. Intermetallics, 2012, 22, 92-98.	1.8	17
701	Temperature and pressure effects on phase stabilities in the Ca–Ge system from first-principles calculations and Debye-Gruneisen model. Intermetallics, 2012, 28, 108-119.	1.8	10
702	Preparation, crystal structure and photoluminescence of lithium magnesium manganese borate solid solutions, LiMg _{1-x} Mn _x BO ₃ . Journal of Alloys and Compounds, 2012, 512, 223-229.	2.8	10
703	Crystal structure determination of solar cell materials: Cu ₂ ZnSnS ₄ thin films using X-ray anomalous dispersion. Journal of Alloys and Compounds, 2012, 524, 22-25.	2.8	43
704	An investigation of the Fe and Mo oxidation states in Sr ₂ Fe _{2-x} Mo _x O ₆ (0.25 $\leq x \leq 1.0$) double perovskites by X-ray absorption spectroscopy. Journal of Alloys and Compounds, 2012, 537, 323-331.	2.8	21
705	Crystal structure and ferroelectric property of Bi ₄ Si ₃ O ₁₂ -added Bi _{4-x} S _m Ti ₃ O ₁₂ . Journal of Physics and Chemistry of Solids, 2012, 73, 1223-1228.	1.9	8
706	Electrochemical behavior of mixed conducting oxide cathode on oxygen excess-type solid electrolyte. Journal of Power Sources, 2012, 217, 170-174.	4.0	11
707	Microstructural investigation of Li _x Ni _{1/3} Mn _{1/3} Co _{1/3} O ₂ ($x \leq 1$) and its aged products via magnetic and diffraction study. Journal of Power Sources, 2012, 220, 405-412.	4.0	61

#	ARTICLE	IF	CITATIONS
708	Structural and electronic properties of the hydrogen storage compound Ca(BH ₄) ₂ ·2NH ₃ from first-principles. Computational Materials Science, 2012, 54, 345-349.	1.4	3
709	Capture Lithium in $\text{Li}^{\pm}\text{MnO}_2$: Insights from First Principles. Chemistry of Materials, 2012, 24, 3943-3951.	3.2	114
710	Structural Properties of Pure and Nickel-Modified Nanocrystalline Tungsten Trioxide. Journal of Physical Chemistry C, 2012, 116, 17029-17039.	1.5	13
711	Linear Band-Gap Modulation of Graphane Nanoribbons under Uniaxial Elastic Strain: A Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 9356-9359.	1.5	32
712	Structure-property relations in hexagonal and monoclinic BiPO ₄ :Eu ³⁺ nanoparticles synthesized by polyol-mediated method. RSC Advances, 2012, 2, 1477-1485.	1.7	61
713	Supramolecular assemblies built from lanthanide ammoniocarboxylates and cucurbit[6]uril. CrystEngComm, 2012, 14, 8128.	1.3	24
714	Structural, elastic, magnetic and electronic properties of 4d perovskite CaTcO ₃ : a DFT+U investigation. Journal of Physics Condensed Matter, 2012, 24, 185401.	0.7	3
715	Crystal structure of pseudojohannite, with a revised formula, Cu ₃ (OH) ₂ [(UO ₂) ₄ (SO ₄) ₂](H ₂ O) ₁₂ . American Mineralogist, 2012, 97, 1796-1803.	0.9	17
716	Chemical State Analysis of Entrapped Nitrogen in Carbon Nanohorns Using Soft X-ray Emission and Absorption Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 6793-6799.	1.5	4
717	Global minimum structure search in Li _x CoO ₂ composition using a hybrid evolutionary algorithm. Physical Chemistry Chemical Physics, 2012, 14, 13095.	1.3	12
718	Structural, electronic and ferroelectric properties of croconic acid crystal: a DFT study. Physical Chemistry Chemical Physics, 2012, 14, 14673.	1.3	39
719	Spiral-Spin-Driven Ferroelectricity in a Multiferroic Delafossite AgFeO_2 . Physical Review Letters, 2012, 109, 097203.	2.9	57
720	Ab initio calculations of structural, optical and thermoelectric properties for CoSb ₃ and ACo ₄ Sb ₁₂ (A=La, Tl and Y) compounds. Computational Materials Science, 2012, 65, 509-519.	1.4	95
721	Reversible electrochemical reaction of CuO with Li in the LiCuO ₂ system. Solid State Ionics, 2012, 225, 611-614.	1.3	13
722	Electronic structure calculations and quantum molecular dynamics simulations of the ionic liquid PP13-TFSI. Solid State Ionics, 2012, 225, 22-25.	1.3	9
723	Electrical conductivity and X-ray diffraction analysis of oxyapatite-type lanthanum silicate and neodymium silicate solid solution. Solid State Ionics, 2012, 225, 443-447.	1.3	5
724	Parallel-sheets model analysis of space charge layer formation at metal/ionic conductor interfaces. Solid State Ionics, 2012, 226, 62-70.	1.3	9
725	Structural changes on cycling Li ₂ FeSiO ₄ polymorphs from DFT calculations. Solid State Ionics, 2012, 228, 19-24.	1.3	20

#	ARTICLE	IF	CITATIONS
726	Conductivity and hydration trends in disordered fluorite and pyrochlore oxides: A study on lanthanum cerate-zirconate based compounds. <i>Solid State Ionics</i> , 2012, 229, 26-32.	1.3	32
727	First principles NMR study of fluorapatite under pressure. <i>Solid State Nuclear Magnetic Resonance</i> , 2012, 45-46, 59-65.	1.5	12
728	Structural refinement and photoluminescence properties of irregular cube-like (Ca _{1-x} Cu _x)TiO ₃ microcrystals synthesized by the microwave-hydrothermal method. <i>Materials Chemistry and Physics</i> , 2012, 136, 130-139.	2.0	24
729	Magnetism in melt grown dilute magnetic semiconductor Ge _{1-x} Mn _x from electron density. <i>Materials Science in Semiconductor Processing</i> , 2012, 15, 731-739.	1.9	2
730	Molecular Dynamics Studies on the Adaptability of an Ionic Liquid in the Extraction of Solid Nanoparticles. <i>Langmuir</i> , 2012, 28, 13924-13932.	1.6	16
731	Thermodynamics of Lithium in TiO ₂ (B) from First Principles. <i>Chemistry of Materials</i> , 2012, 24, 1568-1574.	3.2	90
732	The mechanism for hydrothermal growth of zinc oxide. <i>CrystEngComm</i> , 2012, 14, 1232-1240.	1.3	94
733	New Vanadium Selenites: Centrosymmetric Ca ₂ (VO ₂) ₂ (SeO ₃) ₃ (H ₂ O) ₂ , Sr ₂ (VO ₂) ₂ (SeO ₃) ₃ , and Ba(V ₂ O ₅)(SeO ₃), and Noncentrosymmetric and Polar A ₄ (VO ₂) ₂ (SeO ₃) ₄ (Se ₂ O ₅) (A = Sr ²⁺ or Pb ²⁺). <i>Inorganic Chemistry</i> , 2012, 51, 609-619.	1.9	43
734	Solution synthesis of homogeneous plate-like multifunctional CeO ₂ particles. <i>RSC Advances</i> , 2012, 2, 5976.	1.7	30
735	Possible "type carrier sources in In ₂ O ₃ (ZnO) _k . <i>Chemistry of Materials</i> , 2012, 24, 106-114.	3.2	38
736	First-principles analysis of oxide-ion conduction mechanism in lanthanum silicate. <i>Journal of Materials Chemistry</i> , 2012, 22, 7265.	6.7	29
737	Electronic structure of Ta ₂ NiSe ₅ as a candidate for excitonic insulators. <i>Journal of Physics: Conference Series</i> , 2012, 400, 032035.	0.3	15
738	Orientation Relationships between Directionally Grown Precipitates and their Parent Phases in Steels. <i>Materials Science Forum</i> , 0, 706-709, 61-68.	0.3	1
739	Magnetic and Neutron Diffraction Study on Melilite-Type Oxides Sr ₂ MGe ₂ O ₇ (M = Mn, Co). <i>Inorganic Chemistry</i> , 2012, 51, 3572-3578.	1.9	21
740	H ₂ Ti ₆ O ₁₃ , a new protonated titanate prepared by Li ⁺ /H ⁺ ion exchange: synthesis, crystal structure and electrochemical Li insertion properties. <i>RSC Advances</i> , 2012, 2, 3530.	1.7	31
741	Insight into the channel ion distribution and influence on the lithium insertion properties of hexatitanates A ₂ Ti ₆ O ₁₃ (A = Na, Li, H) as candidates for anode materials in lithium-ion batteries. <i>Dalton Transactions</i> , 2012, 41, 14633.	1.6	44
742	Crystal Structure of Cu-Sn-In Alloys Around the Î-Phase Field Studied by Neutron Diffraction. <i>Journal of Electronic Materials</i> , 2012, 41, 3223-3231.	1.0	10
743	Self-Limiting Growth of Hexagonal and Triangular Quantum Dots on (111)A. <i>Crystal Growth and Design</i> , 2012, 12, 1411-1415.	1.4	44

#	ARTICLE	IF	CITATIONS
744	Predicted Suppression of the Superconducting Transition of New High-Pressure Yttrium Phases with Increasing Pressure from First-Principles Calculations. <i>Physical Review Letters</i> , 2012, 109, 157004.	2.9	31
745	Two-dimensional charge fluctuation in \hat{I}^2 -Na _{0.33} V ₂ O ₅ . <i>Physical Review B</i> , 2012, 85, .	1.1	8
746	Excellent Catalytic Effects of Graphene Nanofibers on Hydrogen Release of Sodium alanate. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10861-10866.	1.5	33
747	First-principles study on the differences of possible ferroelectric behavior and magnetic exchange interaction between Bi ₂ NiMnO ₆ and La ₂ NiMnO ₆ . <i>AIP Advances</i> , 2012, 2, .	0.6	15
748	Spin-induced symmetry breaking in orbitally ordered NiCr ₂ O ₄ and CuCr ₂ O ₄ . <i>Physical Review B</i> , 2012, 85, .	1.1	95
749	Crystal structure and magnetic properties of Sr ₂ Co ₂ Fe ₂ O ₁₀ . <i>Journal of Applied Physics</i> , 2012, 112, 084105.	1.1	20
750	Water Adsorption and Its Effect on the Stability of Low Index Stoichiometric and Reduced Surfaces of Ceria. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7073-7082.	1.5	204
751	First-Principles Assessment of H ₂ S and H ₂ O Reaction Mechanisms and the Subsequent Hydrogen Absorption on the CeO ₂ (111) Surface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2411-2424.	1.5	101
752	High precision electronic charge density determination for L1 ₀ -ordered \hat{I}^3 -TiAl by quantitative convergent beam electron diffraction. <i>Philosophical Magazine</i> , 2012, 92, 4408-4424.	0.7	3
753	Quantum mechanically guided design of Co ₄₃ Fe ₂₀ Ta _{5.5} X _{31.5} (X=B, Si, P, S) metallic glasses. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 175402.	0.7	5
754	Bonding, Ion Mobility, and Rate-Limiting Steps in Deintercalation Reactions with ThCr ₂ Si ₂ -type KNi ₂ Se ₂ . <i>Journal of the American Chemical Society</i> , 2012, 134, 7750-7757.	6.6	51
755	Understanding Fluxes as Media for Directed Synthesis: <i>In Situ</i> Local Structure of Molten Potassium Polysulfides. <i>Journal of the American Chemical Society</i> , 2012, 134, 9456-9463.	6.6	53
756	First-principles calculation of magnetoelastic coefficients and magnetostriction in the spinel ferrites CoFe ₂ O ₄ and NiFe ₂ O ₄ . <i>Physical Review B</i> , 2012, 85, .	1.1	103
757	Adolfpateráite, K ₂ (UO ₂)(SO ₄)(OH)(H ₂ O), a new uranyl sulphate mineral from Jachymov, Czech Republic. <i>American Mineralogist</i> , 2012, 97, 447-454.	0.9	26
758	Origin of the Ferrielectricity and Visible-Light Photocatalytic Activity of Silver Niobate AgNbO ₃ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 24902-24906.	1.5	43
759	Two New Noncentrosymmetric (NCS) Polar Oxides: Syntheses, Characterization, and Structure-Property Relationships in BaMTe ₂ O ₇ (M = Mg ²⁺ or Tj) and Ba ₂ Te ₂ O ₇ . <i>Journal of Applied Physics</i> , 2012, 112, 084105.	1.0	14
760	A Polar Corundum Oxide Displaying Weak Ferromagnetism at Room Temperature. <i>Journal of the American Chemical Society</i> , 2012, 134, 3737-3747.	6.6	73
761	Eu ³⁺ /Tb ³⁺ -codoped Y ₂ O ₃ nanophosphors: Rietveld refinement, bandgap and photoluminescence optimization. <i>Journal Physics D: Applied Physics</i> , 2012, 45, 415102.	1.3	220

#	ARTICLE	IF	CITATIONS
762	Revealing the Surface Reactivity of Zirconia by Periodic DFT Calculations. Journal of Physical Chemistry C, 2012, 116, 6636-6644.	1.5	58
763	Role of Ga ³⁺ and Cu ²⁺ in the High Interstitial Oxide-Ion Diffusivity of Pr ₂ NiO ₄ -Based Oxides: Design Concept of Interstitial Ion Conductors through the Higher-Valence d ¹⁰ Dopant and Jahn–Teller Effect. Chemistry of Materials, 2012, 24, 4100-4113.	3.2	70
764	TiO ₂ as an electrostatic template for epitaxial growth of EuO on MgO(001) by reactive molecular beam epitaxy. Journal of Applied Physics, 2012, 111, 083912.	1.1	8
765	Clamping of Non-180° Domain Walls in Bi-Based Ferroelectric Single Crystals. Transactions of the Materials Research Society of Japan, 2012, 37, 69-72.	0.2	0
766	DFT Study for Growth of <i>m</i> -Plane GaN/ZnO Interfaces. E-Journal of Surface Science and Nanotechnology, 2012, 10, 221-225.	0.1	0
767	A Next-Generation Three-Dimensional Visualization Program VESTA 3. Nihon Kessho Gakkaishi, 2012, 54, 119-120.	0.0	0
768	Structural relations and pseudosymmetries in the andorite homologous series. Journal of Mineralogical and Petrological Sciences, 2012, 107, 226-243.	0.4	13
769	XAFS Measurement System in the Soft X-ray Region for Various Sample Conditions and Multipurpose Measurements. , 2012, , .		0
770	Metastable ultrathin crystal in thermally grown SiO ₂ film on Si substrate. AIP Advances, 2012, 2, .	0.6	5
771	Structure of the new mineral sarrabusite, Pb ₅ CuCl ₄ (SeO ₃) ₄ , solved by manual electron-diffraction tomography. Acta Crystallographica Section B: Structural Science, 2012, 68, 15-23.	1.8	36
772	Doping level of Mn in high temperature grown Zn _{1-x} Mn _x O studied through electronic charge distribution, magnetization, and local structure. Chemical Papers, 2012, 66, .	1.0	8
773	High-temperature properties of lithium tetraborate Li ₂ B ₄ O ₇ . Journal Physics D: Applied Physics, 2012, 45, 175305.	1.3	50
774	P2-type Na _x [Fe _{1/2} Mn _{1/2}]O ₂ made from earth-abundant elements for rechargeable Na-batteries. Nature Materials, 2012, 11, 512-517.	13.3	1,884
775	Band-gap engineering in TiO ₂ -based ternary oxides. Physical Review B, 2012, 85, .	1.1	16
776	First-principles study of phonon properties in magnetic double-layer manganites. Physical Review B, 2012, 86, .	1.1	3
777	Site-Specific Transition Metal Occupation in Multicomponent Pyrophosphate for Improved Electrochemical and Thermal Properties in Lithium Battery Cathodes: A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2012, 134, 11740-11748.	6.6	37
778	First-principles study on the electronic structure and magnetism of layered oxyselenide La ₂ Mn ₂ Se ₂ O ₃ . Journal of Physics Condensed Matter, 2012, 24, 236003.	0.7	0
779	Dangling bonds and magnetism of grain boundaries in graphene. Physical Review B, 2012, 85, .	1.1	57

#	ARTICLE	IF	CITATIONS
780	High-pressure neutron study of the morphotropic lead-zirconate-titanate: Phase transitions in a two-phase system. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	8
781	Geometry, Electronic Structure, and Bonding in CuMCh_2 (M = Sb, Bi; Ch = S, Se): Alternative Solar Cell Absorber Materials?. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7334-7340.	1.5	97
782	Stabilization of highly polarized PbTiO_3 nanoscale capacitors due to in-plane symmetry breaking at the interface. <i>Physical Review B</i> , 2012, 85, .	1.1	11
783	Electronic Band Structure of Exfoliated Titanium- and/or Niobium-Based Oxide Nanosheets Probed by Electrochemical and Photoelectrochemical Measurements. <i>Journal of Physical Chemistry C</i> , 2012, 116, 12426-12433.	1.5	74
784	Structural anisotropy and annealing-induced nanoscale atomic rearrangements in metamict titanite. <i>American Mineralogist</i> , 2012, 97, 1354-1365.	0.9	17
785	A First-Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys. <i>Advanced Engineering Materials</i> , 2012, 14, 530-546.	1.6	54
786	Y:BaZrO_3 Perovskite Compounds I: DFT Study on the Unprotonated and Protonated Local Structures. <i>Chemistry - an Asian Journal</i> , 2012, 7, 1827-1837.	1.7	14
787	Y:BaZrO_3 Perovskite Compounds II: Designing Protonic Conduction by using MD Models. <i>Chemistry - an Asian Journal</i> , 2012, 7, 1838-1844.	1.7	10
788	Sterically Active Electron Pairs in Lead Sulfide? An Investigation of the Electronic and Vibrational Properties of PbS in the Transition Region Between the Rock Salt and the GeTe type Modifications. <i>Chemistry - A European Journal</i> , 2012, 18, 10929-10936.	1.7	35
789	Rapid Lithium Insertion and Location of Mobile Lithium in the Defect Perovskite $\text{Li}_{0.18}\text{Sr}_{0.66}\text{Ti}_{0.5}\text{Nb}_{0.5}\text{O}_3$. <i>ChemPhysChem</i> , 2012, 13, 2293-2296.	1.0	12
790	Crystal Structure, Oxygen Deficiency, and Oxygen Diffusion Path of Perovskite-Type Lanthanum Cobaltites $\text{La}_{0.4}\text{Ba}_{0.6}\text{CoO}_{3-\delta}$ and $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_{3-\delta}$. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5246-5254.	1.5	33
791	^{29}Si NMR in Cement: A Theoretical Study on Calcium Silicate Hydrates. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9755-9761.	1.5	84
792	Depleted brittle mica structure determination in Ba-phlogopite glass-ceramics. <i>Journal of Materials Science</i> , 2012, 47, 5298-5307.	1.7	2
793	Particle morphology, electrical conductivity, crystal and electronic structures of hydrothermally synthesized $(\text{Ce,Sr})\text{PO}_4$. <i>Journal of Materials Science</i> , 2012, 47, 6220-6225.	1.7	2
794	Quasiharmonic Vibrational Properties of TiNiSn from Ab Initio Phonons. <i>Journal of Electronic Materials</i> , 2012, 41, 977-983.	1.0	31
795	Analysis on insulator-metal transition in yttrium doped LSMO from electron density distribution. <i>Bulletin of Materials Science</i> , 2012, 35, 107-118.	0.8	7
796	Enabling the Li-ion conductivity of Li-metal fluorosulphates by ionic liquid grafting. <i>Journal of Solid State Electrochemistry</i> , 2012, 16, 1743-1751.	1.2	17
797	Irregular Electrical Conduction Types in Tin Oxide Thin Films Induced by Nanoscale Phase Separation. <i>Journal of the American Ceramic Society</i> , 2012, 95, 324-327.	1.9	38

#	ARTICLE	IF	CITATIONS
798	Structural refinement, optical and microwave dielectric properties of BaZrO ₃ . <i>Ceramics International</i> , 2012, 38, 2129-2138.	2.3	104
799	New crystal structural families of lanthanide chloride "Alcohol/water complexes. <i>Inorganica Chimica Acta</i> , 2012, 384, 23-28.	1.2	6
800	Local structural arrangements around oxygen and hydrogen-related defects in proton conducting LaP ₃ O ₉ investigated by first principles calculations. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 7995-8003.	3.8	10
801	Linear scaling algorithm of real-space density functional theory of electrons with correlated overlapping domains. <i>Computer Physics Communications</i> , 2012, 183, 1664-1673.	3.0	25
802	Smectite clays as the quasi-templates for platinum electrodeposition. <i>Electrochimica Acta</i> , 2012, 61, 94-106.	2.6	6
803	Preparation of BaTiO films by laser chemical vapor deposition. <i>Materials Chemistry and Physics</i> , 2012, 133, 398-404.	2.0	13
804	First-principles study of bonding, elasticity-relevant and acoustic properties of BaAlBO ₃ F ₂ . <i>Journal of Physics and Chemistry of Solids</i> , 2012, 73, 109-114.	1.9	9
805	Antiferromagnetic phase transition in garnet-type AgCa ₂ Mn ₂ V ₃ O ₁₂ and NaPb ₂ Mn ₂ V ₃ O ₁₂ . <i>Journal of Physics and Chemistry of Solids</i> , 2012, 73, 471-477.	1.9	2
806	Optical spectroscopy and excited state dynamics of CaMoO ₄ :Pr ³⁺ . <i>Journal of Solid State Chemistry</i> , 2012, 185, 136-142.	1.4	35
807	Structures of ordered tungsten- or molybdenum-containing quaternary perovskite oxides. <i>Journal of Solid State Chemistry</i> , 2012, 185, 107-116.	1.4	47
808	Synthesis, crystal structure and photoluminescence of a new Eu-doped Sr containing sialon (Sr _{0.94} Eu _{0.06})(Al _{0.3} Si _{0.7}) ₄ (N _{0.8} O _{0.2}) ₆ . <i>Journal of Solid State Chemistry</i> , 2012, 190, 264-270.	1.4	16
809	Synthesis, crystal structure, and protonation behaviour in solution of the recently-discovered drug metabolite, N ₁ ,N ₁₀ -diacetyltriethylenetetramine. <i>Journal of Molecular Structure</i> , 2012, 1012, 37-42.	1.8	2
810	Variable temperature neutron diffraction study of Bi ₃ ReO ₈ oxide ion conductor. <i>Solid State Ionics</i> , 2012, 217, 46-53.	1.3	9
811	Preparation of LaRuO ₃ films by microwave plasma-enhanced chemical vapor deposition. <i>Thin Solid Films</i> , 2012, 520, 1847-1850.	0.8	3
812	Formation of Cu ₃ BiS ₃ thin films via sulfurization of Bi-Cu metal precursors. <i>Thin Solid Films</i> , 2012, 520, 5165-5171.	0.8	52
813	Hydrogen shallow donors in ZnO and rutile TiO ₂ . <i>Physica B: Condensed Matter</i> , 2012, 407, 1456-1461.	1.3	10
814	Synthesis and photoluminescence investigations of the white light emitting phosphor, vanadate garnet, Ca ₂ NaMg ₂ V ₃ O ₁₂ co-doped with Dy and Sm. <i>Journal of Luminescence</i> , 2012, 132, 293-298.	1.5	69
815	Ab initio and crystal field studies of the Mn ⁴⁺ -doped Ba ₂ LaNbO ₆ double-perovskite. <i>Journal of Luminescence</i> , 2012, 132, 579-584.	1.5	83

#	ARTICLE	IF	CITATIONS
816	Structure and site selective luminescence of sol-gel derived Eu:Sr ₂ SiO ₄ . Journal of Luminescence, 2012, 132, 1329-1338.	1.5	81
817	Lanthanum tetrazinc, LaZn ₄ . Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, i37-i40.	0.4	14
818	Structure of (Ga ₂ O ₃) ₂ (ZnO) ₁₃ and a unified description of the homologous series (Ga ₂ O ₃) ₂ (ZnO) ₂ · n · 1. Acta Crystallographica Section B: Structural Science, 2012, 68, 250-260.	1.8	7
819	Structural Refinement and Photoluminescence Properties of MnWO ₄ Nanorods Obtained by Microwave-Hydrothermal Synthesis. Journal of Inorganic and Organometallic Polymers and Materials, 2012, 22, 264-271.	1.9	41
820	Atoms-in-molecules analysis of the effect of intermolecular interactions on dielectric properties in hydrogen-bonded material 5-bromo-9-hydroxyphenalenone. International Journal of Quantum Chemistry, 2013, 113, 386-392.	1.0	2
821	High-pressure synthesis of noble metal hydrides. Journal of Chemical Physics, 2013, 138, 134507.	1.2	37
822	Effect of local coordination of Mn on Mn-L _{2,3} edge electron energy loss spectrum. Journal of Applied Physics, 2013, 114, .	1.1	21
823	Structure, Phase Transition Behaviors and Electrical Properties of Nd Substituted Aurivillius Polycrystallines Na _{0.5} Nd _x Bi _{2.5} Nb ₂ O ₉ (x = 0.1, 0.2, 0.3, and 0.5). Inorganic Chemistry, 2013, 52, 5045-5054.	1.9	91
824	Combined Experimental and Computational Study of Oxide Ion Conduction Dynamics in Sr ₂ Fe ₂ O ₅ Brownmillerite. Chemistry of Materials, 2013, 25, 3080-3087.	3.2	55
825	The Effect of Synthetic Method and Annealing Temperature on Metal Site Preference in Al ₁ Ga _x FeO ₃ . Inorganic Chemistry, 2013, 52, 8612-8620.	1.9	9
826	Magnetostructural transition, metamagnetism, and magnetic phase coexistence in Co ₁₀ Ge ₃ O ₁₆ . Physical Review B, 2013, 88, .	1.1	5
827	Magnetic and charge derived properties of ball milled dilute magnetic semiconductor Si _{0.98} Mn _{0.02} . Physica B: Condensed Matter, 2013, 426, 71-78.	1.3	3
828	Magnetic Properties of the RbMnPO ₄ Zeolite-ABW-Type Material: A Frustrated Zigzag Spin Chain. Inorganic Chemistry, 2013, 52, 9627-9635.	1.9	15
829	Molecular beam epitaxy of complex oxides. , 2013, , 417-449.		12
830	Synthesis, Crystal Structure and Physical Properties of Ba ₄ Ti ₁₂ O ₂₇ . Key Engineering Materials, 2013, 566, 211-214.	0.4	3
831	High temperature growth, charge distribution and magnetism in Co and Mn co-doped ZnO. Journal of Materials Science: Materials in Electronics, 2013, 24, 2880-2889.	1.1	2
832	Preparation of TiO ₂ thick film by laser chemical vapor deposition method. Journal of Materials Science: Materials in Electronics, 2013, 24, 1758-1763.	1.1	3
833	Na ₄ Co _{2.4} Mn _{0.3} Ni _{0.3} (PO ₄) ₂ P ₂ O ₇ : High potential and high capacity electrode material for sodium-ion batteries. Electrochemistry Communications, 2013, 34, 266-269.	2.3	81

#	ARTICLE	IF	CITATIONS
834	Clathrate Ba ₈ Au ₁₆ P ₃₀ : The “Gold Standard” for Lattice Thermal Conductivity. <i>Journal of the American Chemical Society</i> , 2013, 135, 12313-12323.	6.6	98
835	Na ₄ Co ₃ (PO ₄) ₂ P ₂ O ₇ : A novel storage material for sodium-ion batteries. <i>Journal of Power Sources</i> , 2013, 234, 175-179.	4.0	212
836	Predicting alloy vibrational mode properties using lattice dynamics calculations, molecular dynamics simulations, and the virtual crystal approximation. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	64
837	Formation Principles for Templated Vanadium Selenite Oxalates. <i>Crystal Growth and Design</i> , 2013, 13, 4504-4511.	1.4	22
838	Effect of pressure on the atomic and electronic structure of enstatite MgSiO ₃ : Ab initio calculations. <i>Technical Physics</i> , 2013, 58, 692-695.	0.2	1
839	A New High-Energy Cathode for a Na-Ion Battery with Ultrahigh Stability. <i>Journal of the American Chemical Society</i> , 2013, 135, 13870-13878.	6.6	393
840	Origin of the vanishing critical thickness for ferroelectricity in free-standing PbTiO ₃ ultrathin films from first principles. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	11
841	Morphology, ion impact, and kinetic parameters of swift heavy-ion-induced Y ₂ O ₃ :Dy ³⁺ phosphor. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2013, 210, 1624-1635.	0.8	22
842	Calculation of arrangement of oxygen ions and vacancies in double perovskite GdBaCo ₂ O ₅ + δ by first-principles DFT with Monte Carlo simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10494.	1.3	18
843	Atomistic study of stress-induced switching of 90° ferroelectric domain walls in PbTiO ₃ : size, temperature and structural effect. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2013, 21, 065019.	0.8	4
844	Crystal structures of spin-Jahn-Teller-ordered MgCr ₂ O ₄ and ZnCr ₂ O ₄ . <i>Journal of Physics Condensed Matter</i> , 2013, 25, 326001.	0.7	33
845	Lattice constant anomaly in the Li _{1+x} V _{1-x} O ₂ system near x = 0. <i>Canadian Journal of Physics</i> , 2013, 91, 444-449.	0.4	6
846	Parametrization scheme with accuracy and transferability for tight-binding electronic structure calculations with extended H ^{1/4} ckel approximation and molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2013, 19, 2363-2373.	0.8	4
847	Steric-Induced Layer Flexion in Templated Vanadium Tellurites. <i>Crystal Growth and Design</i> , 2013, 13, 2190-2197.	1.4	11
849	First-principles calculations for the surface termination of Li ₂ TiO ₃ (001) surfaces. <i>Journal of Nuclear Materials</i> , 2013, 442, S705-S709.	1.3	3
850	Role of oxygen vacancies in the resistive switching of SrZrO ₃ for resistance random access memory. <i>Journal of Alloys and Compounds</i> , 2013, 580, 148-151.	2.8	44
851	Insights into the phase diagram of bismuth ferrite from quasiharmonic free-energy calculations. <i>Physical Review B</i> , 2013, 88, .	1.1	50
852	The First Combined Experimental and Theoretical Evaluation of Tetravalent Cation Conduction in a Solid. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4300-4304.	1.0	2

#	ARTICLE	IF	CITATIONS
853	Ba ₄ Mg[Si ₂ N ₆], Ba ₃ Ca ₂ [Si ₂ N ₆] and Ba _{1.6} Sr _{3.4} [Si ₂ N ₆] – Quaternary barium alkaline-earth silicon nitrides containing isolated nitridosilicate anions of [Si ₂ N ₆] ¹⁰⁻ . Journal of Alloys and Compounds, 2013, 555, 320-324.	2.8	18
854	The binding nature of light hydrocarbons on Fe/MOF-74 for gas separation. Physical Chemistry Chemical Physics, 2013, 15, 19644.	1.3	46
855	Artificially imposed hexagonal ferroelectricity in canted antiferromagnetic YFeO ₃ epitaxial thin films. Materials Chemistry and Physics, 2013, 138, 929-936.	2.0	29
856	Direct Evidence of Cation Disorder in Thermoelectric Lead Chalcogenides PbTe and PbS. Advanced Functional Materials, 2013, 23, 5477-5483.	7.8	98
857	Towards new binary compounds: Synthesis of amorphous phosphorus carbide by pulsed laser deposition. Journal of Solid State Chemistry, 2013, 198, 466-474.	1.4	53
858	Relationships among channel topology and atomic displacements in the structures of Pb ₅ (BO ₄) ₃ Cl with B = P (pyromorphite), V (vanadinite), and As (mimetite). American Mineralogist, 2013, 98, 1573-1579.	0.9	18
859	Antiferromagnetic transitions of osmium-containing rare earth double perovskites Ba ₂ LnOsO ₆ (Ln=rare earths). Journal of Solid State Chemistry, 2013, 206, 300-307.	1.4	9
860	Predicting a new photocatalyst and its electronic properties by density functional theory. Journal of Applied Physics, 2013, 114, .	1.1	24
861	Graphene-mediated exchange coupling between a molecular spin and magnetic substrates. Physical Review B, 2013, 88, .	1.1	17
862	Full control of magnetism in a manganite bilayer by ferroelectric polarization. Physical Review B, 2013, 88, .	1.1	46
863	Low-Temperature Nitridation of Manganese and Iron Oxides Using NaNH ₂ Molten Salt. Inorganic Chemistry, 2013, 52, 11787-11791.	1.9	26
864	High-Pressure Synthesis of 5d Cubic Perovskite BaOsO ₃ at 17 GPa: Ferromagnetic Evolution over 3d to 5d Series. Journal of the American Chemical Society, 2013, 135, 16507-16516.	6.6	58
865	An X-ray absorption spectroscopic study of the effect of bond covalency on the electronic structure of Gd ₂ Ti _{2-x} Sn _x O ₇ . Physical Chemistry Chemical Physics, 2013, 15, 10477.	1.3	26
866	Spin-driven bond order in a 15-magnetization plateau phase in the triangular lattice antiferromagnet CuFeO ₂ . Physical Review B, 2013, 88, .	1.1	10
867	Strong Spin-Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. Advanced Functional Materials, 2013, 23, 1864-1872.	7.8	41
868	New Roles for Icosahedral Clusters in Intermetallic Phases: Micelle-like Segregation of Ca-Cd and Cu-Cd Interactions in Ca ₁₀ Cd ₂₇ Cu ₂ . Journal of the American Chemical Society, 2013, 135, 17369-17378.	6.6	22
869	Electronic and magnetic properties of an organic multiferroic: (C ₂ H ₅ NH ₃) ₂ CuCl ₄ . Journal of Magnetism and Magnetic Materials, 2013, 346, 91-95.	1.0	14
870	Effect of A-site cation disorder on oxygen diffusion in perovskite-type Ba _{0.5} Sr _{0.5} Co _{1-x} FexO _{2.5} . Journal of Materials Chemistry A, 2013, 1, 10345.	5.2	22

#	ARTICLE	IF	CITATIONS
871	Magnetoelastic effects in doped Fe $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle \text{P}$. Physical Review B, 2013, 88, .	1.1	40
872	Ion-Exchange Synthesis, Crystal Structure, and Physical Properties of Hydrogen Titanium Oxide H ₂ Ti ₃ O ₇ . Inorganic Chemistry, 2013, 52, 13861-13864.	1.9	35
873	ÄtÄpitem, U(AsO ₃ OH) ₂ ·4H ₂ O, from JÄichymov, Czech Republic: the first natural arsenate of tetravalent uranium. Mineralogical Magazine, 2013, 77, 137-152.	0.6	14
874	Crystal Structure and Thermoelectric Properties of Misfit-Layered Sulfides [Ln ₂ S ₂] p NbS ₂ (Ln=ÄLanthanides). Journal of Electronic Materials, 2013, 42, 1335-1339.	1.0	16
875	Magnetization States of All-Oxide Spin Valves Controlled by Charge-orbital Ordering of Coupled Ferromagnets. Scientific Reports, 2013, 3, 1830.	1.6	36
876	Ion induced modification of bandgap and CIE parameters in Y ₂ O ₃ :Dy ³⁺ phosphor. Ceramics International, 2013, 39, 7693-7701.	2.3	19
877	Alloying effects on mechanical properties of the CuÄZrÄAl bulk metallic glass composites. Computational Materials Science, 2013, 79, 187-192.	1.4	16
878	The phase stability and mechanical properties of NbÄC system: Using first-principles calculations and nano-indentation. Journal of Alloys and Compounds, 2013, 561, 220-227.	2.8	65
879	Graphyne and Graphdiyne: Versatile Catalysts for Dehydrogenation of Light Metal Complex Hydrides. Journal of Physical Chemistry C, 2013, 117, 21643-21650.	1.5	40
880	Structure and Magnetic Properties of the Ä±-NaFeO ₂ -Type Honeycomb Compound Na ₃ Ni ₂ BiO ₆ . Inorganic Chemistry, 2013, 52, 13605-13611.	1.9	65
881	Protonic conduction, crystal and electronic structures of La _{0.9} Ba _{1.1} Ga _{0.95} Mg _{0.05} O ₄ Ä. Solid State Ionics, 2013, 253, 123-129.	1.3	3
882	Theoretical Study of Atomic Fluorine Diffusion through Bulk TiO ₂ Polymorphs. Journal of Physical Chemistry C, 2013, 117, 5855-5860.	1.5	13
883	The electronic structure of organicaÄinorganic hybrid compounds: (NH ₄) ₂ CuCl ₄ , (CH ₃ NH ₃) ₂ CuCl ₄ and (C ₂ H ₅ NH ₃) ₂ CuCl ₄ . Journal of Physics Condensed Matter, 2013, 25, 295502.	0.7	39
884	Recent progress of half-Heusler for moderate temperature thermoelectric applications. Materials Today, 2013, 16, 387-395.	8.3	474
885	Reflectance anisotropy spectroscopy of Si(111)-(Ä) ETQq0 0 0 rgBT /Overlock 10 Tf 50 192 Td (xmlns:mml="http://www.w3.org/2003/11/Math/MathML") and Ag surfaces. Physical Review B, 2013, 87, .	1.1	7
886	Superconductivity in KSn ₂ with the MgZn ₂ -type structure. Journal of the Korean Physical Society, 2013, 63, 475-476.	0.3	4
887	Phase Stability of Post-spinel Compound AMn ₂ O ₄ (A = Li, Na, or Mg) and Its Application as a Rechargeable Battery Cathode. Chemistry of Materials, 2013, 25, 3062-3071.	3.2	108
888	Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La _{1-x} Sr _x FeO _{3-Ä} (Ä = 0, 0.25, 0.50). Chemistry of Materials, 2013, 25, 3011-3019.	3.2	153

#	ARTICLE	IF	CITATIONS
889	Local moments and suppression of antiferromagnetism in correlated Zr ₄ Fe ₄ Si ₇ . Physical Review B, 2013, 88, .	1.1	0
890	Symmetrization driven spin transition in $\hat{\mu}$ -FeOOH at high pressure. Earth and Planetary Science Letters, 2013, 379, 49-55.	1.8	54
891	Novel Refractory Phase, Ta ₇ Si ₂ (SixB ₁ â€“x) ₂ . Inorganic Chemistry, 2013, 52, 11295-11301.	1.9	1
892	Quantification of electronic band gap and surface states on FeS ₂ (100). Surface Science, 2013, 618, 53-61.	0.8	74
893	Origin of Selective Guest-Induced Magnetism Transition in Fe/MOF-74. Journal of Physical Chemistry Letters, 2013, 4, 2530-2534.	2.1	45
894	Na ₂ AgF ₄ : 1D antiferromagnet with unusually short Ag ²⁺ â€“Ag ²⁺ separation. Dalton Transactions, 2013, 42, 2167-2173.	1.6	12
895	Origin of giant spin-lattice coupling and the suppression of ferroelectricity in EuTiO ₃ from first principles. Physical Review B, 2013, 88, .	1.1	45
896	First-Principles Study of Point Defect Formation in AgNbO ₃ . Japanese Journal of Applied Physics, 2013, 52, 09KF08.	0.8	22
897	Uranylâ€“3d block metal ion heterometallic carboxylate complexes including additional chelating nitrogen donors. CrystEngComm, 2013, 15, 6533.	1.3	34
898	Entropies of defect formation in ceria from first principles. Physical Chemistry Chemical Physics, 2013, 15, 15935.	1.3	48
899	Uranylâ€“copper(ii) heterometallic oxalate complexes: coordination polymers and frameworks. Dalton Transactions, 2013, 42, 10551.	1.6	44
900	On the unusual photoluminescence of Eu ³⁺ in $\hat{\mu}$ -Zn ₂ P ₂ O ₇ : a time resolved emission spectrometric and Juddâ€“Ofelt study. RSC Advances, 2013, 3, 20046.	1.7	79
901	Sulfonate Complexes of Actinide Ions: Structural Diversity in Uranyl Complexes with 2-Sulfobenzoate. Inorganic Chemistry, 2013, 52, 435-447.	1.9	67
902	Synthesis Process and Magnetic Characterization of the Novel Aurivillius Ferroelectric Material $\text{Bi}_4\text{Gd}_2\text{Ti}_3\text{Fe}_2\text{O}_{18}$. IEEE Transactions on Magnetics, 2013, 49, 4660-4663.	1.2	1
903	Li _{0.3} V ₂ O ₅ with high lithium diffusion rate: a promising anode material for aqueous lithium-ion batteries with superior rate performance. Journal of Materials Chemistry A, 2013, 1, 5423.	5.2	45
904	Cu ₃ MCh ₃ (M = Sb, Bi; Ch = S, Se) as candidate solar cell absorbers: insights from theory. Physical Chemistry Chemical Physics, 2013, 15, 15477.	1.3	71
905	Mn ₂ FeSbO ₆ : A ferrimagnetic ilmenite and an antiferromagnetic perovskite. Physical Review B, 2013, 87, .	1.1	31
906	Mechanism of Ferroelectricity in Half-Doped Manganites with Pseudocubic and Bilayer Structure. Journal of the Physical Society of Japan, 2013, 82, 113703.	0.7	11

#	ARTICLE	IF	CITATIONS
907	Investigation of the structure and properties of rhombohedral Cu ²⁺ Ge ²⁺ Te alloys by ab initio calculations. <i>Intermetallics</i> , 2013, 32, 292-296.	1.8	15
908	Synthesis and crystal structure of Mg _{0.5} NbO ₂ : An ion-exchange reaction with Mg ²⁺ between trigonal [NbO ₂] ²⁺ layers. <i>Journal of Solid State Chemistry</i> , 2013, 197, 471-474.	1.4	4
909	Hybrid functional calculation of electronic and phonon structure of BaSnO. <i>Journal of Solid State Chemistry</i> , 2013, 197, 134-138.	1.4	42
910	An investigation of the electronic structure of Cu ₂ FeSn ₃ Ti ₈ (O ₃) thiospinel spin-crossover materials by X-ray absorption spectroscopy and electronic structure calculations. <i>Journal of Solid State Chemistry</i> , 2013, 197, 532-542.	1.4	1
911	An X-ray absorption spectroscopic study of the metal site preference in Al _{1-x} Ga _x FeO ₃ . <i>Journal of Solid State Chemistry</i> , 2013, 197, 147-153.	1.4	18
912	Atomic Structure and Composition of Pt ₃ Co Nanocatalysts in Fuel Cells: An Aberration-Corrected STEM HAADF Study. <i>Chemistry of Materials</i> , 2013, 25, 530-535.	3.2	39
913	Sr ²⁺ fresnoite determined from synchrotron X-ray powder diffraction data. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013, 69, i1-i1.	0.2	7
914	Lithium-Stuffed Diamond Polytype Zn ₃ Tt Structures (Tt = Sn, Ge): The Two Lithium-Zinc Tetrelides Li ₃ Zn ₂ Sn ₄ and Li ₂ ZnGe ₃ . <i>Inorganic Chemistry</i> , 2013, 52, 2809-2816.	1.9	16
915	Effects of strain on ferroelectric polarization and magnetism in orthorhombic HoMnO ₃ . <i>Physical Review B</i> , 2013, 87, .	1.1	17
916	Structural transformation of a lithium-rich Li _{1.2} Co _{0.1} Mn _{0.55} Ni _{0.15} O ₂ cathode during high voltage cycling resolved by in situ X-ray diffraction. <i>Journal of Power Sources</i> , 2013, 229, 239-248.	4.0	472
917	DFT calculations of carbon monoxide adsorbed on anatase TiO ₂ (101) and (001) surfaces: correlation between the binding energy and the CO stretching frequency. <i>Molecular Simulation</i> , 2013, 39, 245-249.	0.9	7
918	Imaging of internal stress around a mineral inclusion in a sapphire crystal: application of micro-Raman and photoluminescence spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2013, 44, 147-154.	1.2	20
919	Substrate-Induced Symmetry Breaking in Silicene. <i>Physical Review Letters</i> , 2013, 110, 076801.	2.9	358
920	Calorimetric study and simulation of the adsorption of methanol and propanol onto activated carbon fibers. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2013, 419, 100-112.	2.3	9
921	Electron density distribution and crystal structure of 27R-AlON, Al ₉ O ₃ N ₇ . <i>Journal of Solid State Chemistry</i> , 2013, 204, 21-26.	1.4	20
922	Magnetic properties and structural transitions of fluorite-related rare earth osmates Ln ₃ O ₅ O ₇ (Ln=Pr, Tb). <i>Journal of Solid State Chemistry</i> , 2013, 198, 176-185.	1.4	22
923	Molecular modeling of adsorbed NDMA and water in MFI zeolites. <i>Microporous and Mesoporous Materials</i> , 2013, 182, 198-206.	2.2	8
924	A novel yellow-emitting SrAlSi ₄ N ₇ :Ce ³⁺ phosphor for solid state lighting: Synthesis, electronic structure and photoluminescence properties. <i>Journal of Solid State Chemistry</i> , 2013, 208, 50-57.	1.4	37

#	ARTICLE	IF	CITATIONS
925	Visualization of conduction pathways in lithium superionic conductors: Li ₂ S-P ₂ S ₅ glasses and Li ₇ P ₃ S ₁₁ glass-ceramic. <i>Chemical Physics Letters</i> , 2013, 584, 113-118.	1.2	40
926	Fluorescence lifetime and Judd-Ofelt parameters of Eu ³⁺ doped SrBPO ₅ . <i>Physica B: Condensed Matter</i> , 2013, 410, 141-146.	1.3	72
927	Designing new n=2 Sillen-Aurivillius phases by lattice-matched substitutions in the halide and [Bi ₂ O ₂] ²⁺ layers. <i>Journal of Solid State Chemistry</i> , 2013, 205, 165-170.	1.4	17
928	Synthesis and Crystal Structures of Ca ₄ SiN ₄ and New Polymorph of Ca ₅ Si ₂ N ₆ . <i>Inorganic Chemistry</i> , 2013, 52, 5559-5563.	1.9	17
929	Spiral-Type Heteropolyhedral Coordination Network Based on Single-Crystal LiSrPO ₄ : Implications for Luminescent Materials. <i>Chemistry - A European Journal</i> , 2013, 19, 15358-15365.	1.7	14
930	Octahedral engineering of orbital polarizations in charge transfer oxides. <i>Physical Review B</i> , 2013, 87, .	1.1	27
931	Muon-spin relaxation study on Li- and Na-diffusion in solids. <i>Physica Scripta</i> , 2013, 88, 068509.	1.2	69
932	Ion Diffusion in Solids Probed by Muon-Spin Spectroscopy. <i>Journal of the Physical Society of Japan</i> , 2013, 82, SA023.	0.7	21
933	Adsorption mechanism of chlorides on carbon nanotubes based on first-principles calculations. <i>Chemical Physics Letters</i> , 2013, 580, 94-98.	1.2	13
934	First-principles study of alkali metal-graphite intercalation compounds. <i>Journal of Power Sources</i> , 2013, 243, 585-587.	4.0	336
935	Crystal structure and magnetic properties and Zn substitution effects on the spin-chain compound Sr ₃ Co ₂ O ₆ . <i>Journal of Solid State Chemistry</i> , 2013, 204, 40-46.	1.4	4
936	Fergusonite-type CeNbO ₄ : Single crystal growth, symmetry revision and conductivity. <i>Journal of Solid State Chemistry</i> , 2013, 204, 291-297.	1.4	25
937	Donor/acceptor neutral aggregation of a paddlewheel-type [Ru ₂ II,II] complex and TCNQ. <i>Polyhedron</i> , 2013, 52, 1213-1218.	1.0	7
938	Ferromagnetism on surface of YBa ₂ Cu ₃ O ₇ particle. <i>Physica C: Superconductivity and Its Applications</i> , 2013, 492, 80-89.	0.6	6
939	New germanide superconductors with the type-I clathrate type structure. <i>Physica C: Superconductivity and Its Applications</i> , 2013, 494, 74-76.	0.6	1
940	Structural and electrochemical properties of hydrogen titanium oxides. <i>Solid State Ionics</i> , 2013, 252, 109-115.	1.3	9
941	Local structure analysis on (La,Ba)(Ga,Mg)O ₃ by the pair distribution function method using a neutron source and density functional theory calculations. <i>Solid State Communications</i> , 2013, 163, 46-49.	0.9	5
942	Investigation of CHBrF ₂ adsorbed on TiO ₂ through IR spectroscopy and DFT calculations. <i>Vibrational Spectroscopy</i> , 2013, 65, 142-146.	1.2	3

#	ARTICLE	IF	CITATIONS
943	Brønsted acid–base reactions with anhydrous sulfamates as a pathway to [SO ₃ N]3 ⁻ -containing compounds: Preparation of Li ₃ SO ₃ N. <i>Solid State Sciences</i> , 2013, 25, 28-32.	1.5	5
944	Synthesis, Structure, and Characterization of Two New Polar Sodium Tungsten Selenites: Na ₂ (WO ₃) ₃ (SeO ₃) ₂ ·2H ₂ O and Na ₆ (W ₆ O ₁₉)(SeO ₃) ₂ . <i>Inorganic Chemistry</i> , 2013, 52, 2637-2647.	1.9	44
945	The crystal structure of magnesiozippeite, Mg[(UO ₂) ₂ O ₂ (SO ₄)](H ₂ O) _{3.5} , from East Saddle Mine, San Juan County, Utah (U.S.A.). <i>Mineralogy and Petrology</i> , 2013, 107, 211-219.	0.4	13
946	Building multi-component crystals from cations and co-crystals: the use of chaperones. <i>CrystEngComm</i> , 2013, 15, 2241-2250.	1.3	12
947	Concerted Migration Mechanism in the Li Ion Dynamics of Garnet-Type Li ₇ La ₃ Zr ₂ O ₁₂ . <i>Chemistry of Materials</i> , 2013, 25, 425-430.	3.2	206
948	Structural domain walls in polar hexagonal manganites. <i>Nature Communications</i> , 2013, 4, 1540.	5.8	103
949	Charge density wave fluctuations, heavy electrons, and superconductivity in KNi ₂ S ₂ . <i>Physical Review B</i> , 2013, 87, .	1.1	42
950	One- to three-dimensional uranyl–organic assemblies with 3-sulfophthalic and 5-sulfoisophthalic acids. <i>CrystEngComm</i> , 2013, 15, 2401.	1.3	28
951	Structural, Electronic, and Ferroelectric Properties of Compressed CdPbO ₃ Polymorphs. <i>Inorganic Chemistry</i> , 2013, 52, 1032-1039.	1.9	14
952	Raman enhancement by plasmonic excitation of structurally-characterized metal clusters: Au ₈ , Ag ₈ , and Cu ₈ . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5424.	1.3	12
953	Effect of Co Doping on the Properties of ZnO Bulk Samples. <i>Journal of Electronic Materials</i> , 2013, 42, 701-710.	1.0	6
954	Structural and correlation effects in the itinerant insulating antiferromagnetic perovskite NaOsO ₃ . <i>Physical Review B</i> , 2013, 87, .	1.1	35
955	Electronic states of intrinsic surface and bulk vacancies in FeS ₂ . <i>Journal of Physics Condensed Matter</i> , 2013, 25, 045004.	0.7	35
956	<i>Ab initio</i> analysis of the defect structure of ceria. <i>Physical Review B</i> , 2013, 87, .	1.1	125
957	Ferromagnetic ordering with Heavy Fermion behavior in YbPdSi. <i>Solid State Communications</i> , 2013, 159, 65-69.	0.9	15
958	Computationally Assisted Identification of Functional Inorganic Materials. <i>Science</i> , 2013, 340, 847-852.	6.0	62
959	Anomalous Manganese Activation of a Pyrophosphate Cathode in Sodium Ion Batteries: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 2787-2792.	6.6	165
960	BaFe ₉ LiO ₁₅ : A New Layered Antiferromagnetic Ferrite. <i>Inorganic Chemistry</i> , 2013, 52, 4866-4872.	1.9	3

#	ARTICLE	IF	CITATIONS
961	An investigation of pyrochlore-type oxides ($\text{Yb}_2\text{Ti}_2\text{O}_7$) by XANES. <i>Journal of Physics and Chemistry of Solids</i> , 2013, 74, 830-836.	1.9	16
962	Crystallographic Correlations with Anisotropic Oxide Ion Conduction in Aluminum-Doped Neodymium Silicate Apatite Electrolytes. <i>Chemistry of Materials</i> , 2013, 25, 1109-1120.	3.2	18
963	Reactive surface area of the $\text{Li}_x(\text{Co}_{1/3}\text{Ni}_{1/3}\text{Mn}_{1/3})\text{O}_2$ electrode determined by $\text{H}^{1/4}+\text{SR}$ and electrochemical measurements. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10402.	1.3	31
964	Manipulation of Phase and Microstructure at Nanoscale for SiC in Molten Salt Synthesis. <i>Chemistry of Materials</i> , 2013, 25, 2021-2027.	3.2	45
965	Theoretical Prediction of Multiferroicity in $\text{SmBaMn}_2\text{O}_6$. <i>Journal of the Physical Society of Japan</i> , 2013, 82, 043702.	0.7	15
966	X-ray photoelectron diffraction study of dopant effects in $\text{La}_{0.7}\text{X}_{0.3}\text{MnO}_3$ (X = La, Sr, Ca, Ce) thin films. <i>Journal of Applied Physics</i> , 2013, 113, 063511.	1.1	10
967	Complexation of Uranyl and Rare-Earth Ions by a Fluorinated Tetracarboxylate. Formation of a Layered Assembly and Three-Dimensional Frameworks. <i>Crystal Growth and Design</i> , 2013, 13, 3216-3224.	1.4	34
968	Application of the condensed Fukui function to predict reactivity in core-shell transition metal nanoparticles. <i>Electrochimica Acta</i> , 2013, 101, 334-340.	2.6	31
969	$\text{NaFe}_{0.5}\text{Co}_{0.5}\text{O}_2$ as high energy and power positive electrode for Na-ion batteries. <i>Electrochemistry Communications</i> , 2013, 34, 60-63.	2.3	262
970	Experimental visualization of the Bi-O covalency in ferroelectric bismuth ferrite (BiFeO_3) by synchrotron X-ray powder diffraction analysis. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6779.	1.3	49
971	Environment-mediated structure, surface redox activity and reactivity of ceria nanoparticles. <i>Nanoscale</i> , 2013, 5, 6063.	2.8	71
972	Pd^{2+} -Incorporated Perovskite $\text{CaPd}_3\text{B}_4\text{O}_{12}$ (B = Ti, V). <i>Inorganic Chemistry</i> , 2013, 52, 1604-1609.	1.9	43
973	Raman scattering study of MgH_2 and MgD_2 . <i>Solid State Communications</i> , 2013, 154, 77-80.	0.9	13
974	2,2'-Bipyridine and 1,10-Phenanthroline as Coligands or Structure-Directing Agents in Uranyl-Organic Assemblies with Polycarboxylic Acids. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4563-4573.	1.0	55
975	Europium-Activated K_2SrPO_4 (Ba , Sr) Solid Solutions as Color-Tunable Phosphors for Near-UV Light-Emitting Diode Applications. <i>Journal of the American Ceramic Society</i> , 2013, 96, 1526-1532.	1.9	22
976	Structure and magnetism of disordered carbon. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 255301.	0.7	0
977	Electronic Phase Transition and an Anomalous Ordered Phase in $\text{Ba}_2\text{Ti}_3\text{O}_{22}$ with 3d Ions on a Triangle-Based Lattice. <i>Physical Review Letters</i> , 2013, 110, 196405.	2.9	2
978	MEM Charge Density Study of Olivine LiMPO_4 and MPO_4 (M = Mn, Fe) as Cathode Materials for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2608-2615.	1.5	23

#	ARTICLE	IF	CITATIONS
979	Elucidating the Nature of Pseudo Jahnâ€Teller Distortions in LiMnPO_4 : Combining Density Functional Theory with Soft and Hard X-ray Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2013, 117, 10383-10396.	1.5	72
980	Synthesis and crystal chemistry of the hybrid perovskite $(\text{CH}_3\text{NH}_3)\text{PbI}_3$ for solid-state sensitised solar cell applications. <i>Journal of Materials Chemistry A</i> , 2013, 1, 5628.	5.2	2,254
981	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. <i>American Mineralogist</i> , 2013, 98, 752-759.	0.9	55
982	Location of CO_2 on silicalite-1 zeolite using a single-crystal X-ray method. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2013, 228, 180-186.	0.4	12
983	Spin switching and magnetization reversal in single-crystal NdFeO_3 . <i>Physical Review B</i> , 2013, 87, .	1.1	166
984	Swift heavy ion induced structural and optical properties of $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ nanophosphor. <i>Materials Research Bulletin</i> , 2013, 48, 844-851.	2.7	51
985	Structural mechanism for ultrahigh-strength Co-based metallic glasses. <i>Scripta Materialia</i> , 2013, 68, 257-260.	2.6	12
986	In-situ transmission electron microscopy and first-principles study of Au (100) surface dislocation dynamics. <i>Surface Science</i> , 2013, 608, 154-164.	0.8	5
987	A Unique Approach to Characterization of Solâ€Gelâ€Derived Rareâ€Earthâ€Doped Oxyfluoride Glassâ€Ceramics. <i>Journal of the American Ceramic Society</i> , 2013, 96, 476-480.	1.9	12
988	<i>B</i> -Site Deficiencies in <i>A</i> -site-Ordered Perovskite $\text{LaCu}_3\text{Pt}_{3.75}\text{O}_{12}$. <i>Inorganic Chemistry</i> , 2013, 52, 3985-3989.	1.9	12
989	Suppression of Intersite Charge Transfer in Charge-Disproportionated Perovskite $\text{YCu}_3\text{Fe}_4\text{O}_{12}$. <i>Journal of the American Chemical Society</i> , 2013, 135, 6100-6106.	6.6	40
990	An atomistic description of the high-field degradation of dielectric polyethylene. <i>Journal of Chemical Physics</i> , 2013, 139, 174904.	1.2	31
991	Insights into the Mechanism of Fe(II) Adsorption and Oxidation at Feâ€Clay Mineral Surfaces from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 22880-22886.	1.5	53
992	Selective NO Trapping in the Pores of Chain-Type Complex Assemblies Based on Electronically Activated Paddlewheel-Type $[\text{Ru}_2^{\text{II,II}}]/[\text{Rh}_2^{\text{II,II}}]$ Dimers. <i>Journal of the American Chemical Society</i> , 2013, 135, 18469-18480.	6.6	47
993	Chemical ordering rather than random alloying in SbAs. <i>Physical Review B</i> , 2013, 87, .	1.1	14
994	Modulation of the work function of fullerenes C_{60} and C_{70} by alkali-metal adsorption: A theoretical study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 2676-2680.	0.9	9
995	Effect of $\text{MgO}(100)$ support on structure and properties of Pd and Pt nanoparticles with 49-155 atoms. <i>Journal of Chemical Physics</i> , 2013, 139, 084701.	1.2	41
996	Superatomic Crystal Clusters in Transition Metal Oxides: Molybdenum hollandite $\text{K}_2\text{Mo}_8\text{O}_{16}$. <i>Physical Review B</i> , 2013, 87, .	1.1	5

#	ARTICLE	IF	CITATIONS
997	Control of magnetic interaction and ferroelectricity by nonmagnetic Ga substitution in multiferroic YMn ₂ O ₇ . Physical Review B, 2013, 87, .	1.1	9
998	Novel alkaline earth copper germanates with ferro and antiferromagnetic S=1/2 chains. Journal of Solid State Chemistry, 2013, 198, 39-44.	1.4	9
999	Magnetic structures of Mn ₃ Fe ₂ Sn ₂ O ₁₂ . Physical Review B, 2013, 87, .	1.1	7
1000	MnO ₂ probed by neutron diffraction. Physical Review B, 2013, 87, .	1.1	37
1001	Tetrahedral Framework Structures: Polymorphic Phase Transition with Reorientation of Hexagonal Helical Channels in the Zintl Compound Na ₂ ZnSn ₅ and Its Relation to Na ₅ Zn ₂ +xSn ₁₀ â€“x. Journal of the American Chemical Society, 2013, 135, 10654-10663.	6.6	10
1002	The bis(ethylenedithio)tetrathiafulvalene-based ionic charge-transfer complex with 2,3-dichloro-5,6-dicyano- <i>p</i> -benzoquinone. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 400-402.	0.4	1
1003	Phase analysis in Zn _{1-x} CrxO through charge density. Phase Transitions, 2013, 86, 620-632.	0.6	1
1004	Observation of a kink during the formation of the Kondo resonance band in a heavy-fermion system. Physical Review B, 2013, 88, .	1.1	15
1005	Ferroelectric ground state and polarization-switching path of orthorhombic YMnO ₃ with coexisting E-type and cycloidal spin phases. Physical Review B, 2013, 88, .	1.1	6
1006	Extending Hirshfeldâ€™s to bulk and periodic materials. Journal of Computational Chemistry, 2013, 34, 405-417.	1.5	72
1007	Weak localization and Mott state in two-dimensional Sr ₃ V ₅ S ₁₁ . Journal of Physics Condensed Matter, 2013, 25, 435604.	0.7	2
1008	Åvenekite, Ca[AsO ₂ (OH) ₂] ₂ , a new mineral from JÃ¡chymov, Czech Republic. Mineralogical Magazine, 2013, 77, 2711-2724.	0.6	6
1009	Paratacamite-(Mg), Cu ₃ (Mg,Cu)Cl ₂ (OH) ₆ ; a new substituted basic copper chloride mineral from Camerones, Chile. Mineralogical Magazine, 2013, 77, 3113-3124.	0.6	17
1010	Structural Analysis and Superconducting Properties of F-Substituted NdOBiS ₂ Single Crystals. Journal of the Physical Society of Japan, 2013, 82, 113701.	0.7	94
1011	Validation of density functionals for transition metals and intermetallics using data from quantitative electron diffraction. Journal of Chemical Physics, 2013, 138, 084504.	1.2	6
1012	Comparison between Gaussian-type orbitals and plane wave <i>ab initio</i> density functional theory modeling of layer silicates: Talc [Mg ₃ Si ₄ O ₁₀ (OH) ₂] as model system. Journal of Chemical Physics, 2013, 139, 204101.	1.2	44
1013	Investigation of Mn adatoms adsorption on graphene using first-principles calculation. Journal of Physics: Conference Series, 2013, 417, 012003.	0.3	0
1014	First-Principles Modeling for Current-Voltage Characteristics of Resistive Random Access Memories. Materials Research Society Symposia Proceedings, 2013, 1562, 1.	0.1	0

#	ARTICLE	IF	CITATIONS
1015	Electron density distribution and crystal structure of $21R\text{-AlON}$, $\text{Al}_7\text{O}_3\text{N}_5$. Powder Diffraction, 2013, 28, 171-177.	0.4	16
1016	Polar and Magneto-Electric Properties of Anti-Ferrodistoritive Ordered Jahn-Teller Distortions in a multiferroic metal-organic framework. Journal of Physics: Conference Series, 2013, 428, 012029.	0.3	15
1017	Crystal Structural Analyses of Ferrielectric Tetragonal $(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3 \approx 7\% \text{BaTiO}_3$ Powders and Single Crystals. Japanese Journal of Applied Physics, 2013, 52, 09KD01.	0.8	26
1018	Ab initio evaluation of oxygen diffusivity in LaFeO_3 : the role of lanthanum vacancies. MRS Communications, 2013, 3, 161-166.	0.8	26
1019	Structure and Electrochemical Properties of O3-Type Layered $\text{Li}_{1-x}\text{Mn}_{0.5}\text{Ni}_{0.25}\text{Ti}_{0.25}\text{O}_2$ Prepared by Ion-Exchange. Key Engineering Materials, 0, 566, 123-126.	0.9	10
1020	A first-principles study of the structural and elastic properties of orthorhombic and tetragonal $\text{Ca}_3\text{Mn}_2\text{O}_7$. Chinese Physics B, 2013, 22, 066201.	0.7	6
1021	Relationship between Ferroelectric Performance, Crystal and Electronic Structures in $\text{SrBi}_2(\text{Ta}_{1-x}\text{Nb}_x)_{1.95}\text{M}_{0.05}\text{O}_9$ (M) $T_{FE} \propto 0.00 \text{rgBT} / \text{Ov}$	1.9	19
1022	SOWOS: an open-source program for the three-dimensional Wulff construction. Journal of Applied Crystallography, 2013, 46, 811-816.	1.9	19
1023	Structural phase transition in $\text{Zn}_{1.98}\text{Mn}_{0.02}\text{P}_2\text{O}_7$: EPR evidence for enhanced line broadening and large zero-field splitting parameter in high temperature phase. Journal of Materials Research, 2013, 28, 3157-3163.	1.2	3
1024	Electronic correlation effects in the Cr_2GeC $M_{i>n+1}AX_{i>x}$ phase. Journal of Physics Condensed Matter, 2013, 25, 035601.	0.7	34
1025	Improvement of Cycling Stability at 80°C for 4 V-Class Lithium-Ion Batteries and Safety Evaluation. Journal of the Electrochemical Society, 2013, 160, A1311-A1318.	1.3	7
1026	Molecular dynamics study of network statistics in lithium disilicate: $\langle i>Q</i>n$ distribution and the pressure-volume diagram. Journal of Chemical Physics, 2013, 139, 064503.	1.2	15
1027	Phonon anomalies and lattice dynamics in the superconducting oxychlorides $\text{Ca}_2\text{CuO}_2\text{Cl}_2$. Physical Review B, 2013, 88, .	1.1	13
1028	Cluster-packing geometry for Al-based F-type icosahedral alloys. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, 322-340.	0.3	27
1029	Mode-selective electron-phonon coupling in laser photoemission on $\text{Cu}(110)$. Physical Review B, 2013, 88, .	1.1	6
1030	Epilayer thickness and strain dependence of $\text{Ge}(113)$ surface energies. Physical Review B, 2013, 87, .	1.1	10
1031	Raman and IR reflection microspectroscopic study of Er:YAG laser treated permanent and deciduous human teeth. Journal of Raman Spectroscopy, 2013, 44, 1483-1490.	1.2	19
1032	Ideal design of textured LiCoO_2 sintered electrode for Li-ion secondary battery. APL Materials, 2013, 1, .	2.2	20

#	ARTICLE	IF	CITATIONS
1033	Atomic scattering spectroscopy for determination of the polarity of semipolar AlN grown on ZnO. Applied Physics Letters, 2013, 103, .	1.5	5
1034	Visualization of Bi ³⁺ off-centering in the average cubic structure of (Ba _{0.70} Bi _{0.30})(Ti _{0.70} Fe _{0.30})O ₃ at the electron density level. Applied Physics Letters, 2013, 103, .	1.5	13
1035	Partially disordered spin structure in Ag ₂ CrO ₂ studied with thermodynamic stability of alkali-metal zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	8
1036	Thermodynamic stability of alkali-metal zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
1037	Adsorption and Electronic Structure of Sr and Ag Atoms on Graphite Surfaces: a First-Principles Study. Chinese Physics Letters, 2013, 30, 066801.	1.3	4
1038	Factors for Improvements of Catalytic Activity of Zirconium Oxide-Based Oxygen-Reduction Electrocatalysts. Journal of the Electrochemical Society, 2013, 160, F162-F167.	1.3	36
1039	Preparation and dielectric property of (Li _{0.12} Na _{0.88})NbO ₃ -based solid solutions. Journal of the Ceramic Society of Japan, 2013, 121, 544-549.	0.5	0
1040	Morphology and surface structure of cubic BaTiO ₃ using first-principles density functional theory. Journal of the Ceramic Society of Japan, 2013, 121, 611-613.	0.5	9
1041	Direct observation of negative thermal expansion in SrCu ₃ Fe ₄ O ₁₂ . Journal of the Ceramic Society of Japan, 2013, 121, 912-914.	0.5	10
1042	Residual-Charge Induced Memory Effect of Electric Polarization in Multiferroic CuFe _{1-x} Ga _x O ₂ as Seen via Polarized Neutron Diffraction. Journal of the Physical Society of Japan, 2013, 82, 024706.	0.7	7
1043	Pressure-Induced Superconductivity in Mineral Calaverite AuTe ₂ . Journal of the Physical Society of Japan, 2013, 82, 113704.	0.7	25
1044	Analysis of Molecular Motion of Proton-conductive Imidazolium Hydrogen Succinate Crystal Using Solid-state NMR. Chemistry Letters, 2013, 42, 1323-1325.	0.7	11
1045	Chemical Inhomogeneity, Short-Range Order, and Magnetism in the LiNiO ₂ –NiO Solid Solution. Chemistry - A European Journal, 2013, 19, 14521-14531.	1.7	22
1046	Syntheses and crystal structures of Li(Ta _{0.89} Ti _{0.11})O _{2.945} and (Li _{0.977} Eu _{0.023})(Ta _{0.89} Ti _{0.11})O _{2.968} . Powder Diffraction, 2013, 28, 178-183.	0.4	8
1047	Synchrotron X-ray powder diffraction study on synthetic Sr-Fresnoite. Powder Diffraction, 2013, 28, S333-S338.	0.4	3
1048	Frequency of Filler Vibrations in CoSb ₃ Skutterudites: A Mechanical Interpretation. Journal of the Physical Society of Japan, 2013, 82, 014602.	0.7	7
1049	The observation of scintillation in a hydrated inorganic compound: CeCl ₃ ·6H ₂ O. Applied Physics Letters, 2013, 103, 141909.	1.5	4
1050	Oxide-Ion Conduction, Average and Local Structures of LaSrGa _{1-x} Mg _x O ₄ with Layered Perovskite Structure. Electrochemistry, 2013, 81, 448-453.	0.6	14

#	ARTICLE	IF	CITATIONS
1051	Substitution Effect on Cathode Property, Crystal and Electronic Structures of LiMn _{0.5} Ni _{0.5} O ₂ as Cathode Active Material for Li-Ion Battery. <i>Electrochemistry</i> , 2013, 81, 971-976.	0.6	1
1052	Synthesis, structure and properties of new functional oxynitride ceramics. <i>Journal of the Ceramic Society of Japan</i> , 2013, 121, 142-149.	0.5	11
1053	Energetic Stability and Thermoelectric Property of Alkali-Metal-Encapsulated Type-I Silicon-Clathrate from First-Principles Calculation. <i>Materials Transactions</i> , 2013, 54, 276-285.	0.4	16
1054	Iseite, Mn ₂ Mo ₃ O ₈ , a new mineral from Ise, Mie Prefecture, Japan. <i>Journal of Mineralogical and Petrological Sciences</i> , 2013, 108, 37-41.	0.4	4
1055	A new (2 Å ⁻¹) reconstructed edge structure of zigzag Si nanoribbon: First principles study. <i>Journal of Chemical Physics</i> , 2013, 139, 104703.	1.2	13
1056	High-Pressure Synthesis of Novel Transition Metal Oxides Containing Unusual High Valence Ions. <i>Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu</i> , 2013, 23, 167-173.	0.1	1
1057	Compression behavior of manganite. <i>Journal of Mineralogical and Petrological Sciences</i> , 2013, 108, 295-299.	0.4	9
1058	Chemical Substitution Effect on CDW State in LaAgSb ₂ . , 2014, , .		5
1059	Li-Ion Dynamics in Li _{5+x} La ₃ Zr _x Nb ₂ â ⁺ xO ₁₂ . , 2014, , .		1
1060	Reactive sintering of pseudobrookite-type MgFeNbO ₅ and MgFeTaO ₅ ceramics. <i>IOP Conference Series: Materials Science and Engineering</i> , 2014, 54, 012011.	0.3	2
1061	Layered oxides as positive electrode materials for Na-ion batteries. <i>MRS Bulletin</i> , 2014, 39, 416-422.	1.7	208
1062	Modulating magnetism of nitrogen-doped zigzag graphene nanoribbons. <i>Chinese Physics B</i> , 2014, 23, 067305.	0.7	7
1063	Fluorinated graphene and hexagonal boron nitride as ALD seed layers for graphene-based van der Waals heterostructures. <i>Nanotechnology</i> , 2014, 25, 355202.	1.3	5
1064	Tunable luminescence of Bi ³⁺ -doped YP _x V _{1-â⁺} xO ₄ (0 â%â) Tj ETQq1 1 0,784314 36	0.7	36
1065	Enhanced Performance of Aqueous Sodium-Ion Batteries Using Electrodes Based on the NaTi ₂ (PO ₄) ₃ /MWNTsâ ⁺ Na _{0.44} MnO ₂ System. <i>Energy Technology</i> , 2014, 2, 705-712.	1.8	56
1066	band gap of the hybrid organic-inorganic perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ Effect of spin-orbit interaction, semicore electrons, and. <i>Physical Review B</i> , 2014, 89,	1.1	126
1067	Preparation of (100)-oriented CeO ₂ film on (100) MgO single crystal substrate by laser chemical vapor deposition using solid precursor. <i>Ceramics International</i> , 2014, 40, 15919-15923.	2.3	15
1068	An investigation of the electronic structure and structural stability of RE ₂ Ti ₂ O ₇ by glancing angle and total electron yield XANES. <i>Journal of Alloys and Compounds</i> , 2014, 616, 516-526.	2.8	11

#	ARTICLE	IF	CITATIONS
1069	Origin of major donor states in InGaZn oxide. Journal of Applied Physics, 2014, 116, .	1.1	43
1070	Site engineering concept of Ce ³⁺ -activated novel orange-red emission oxide phosphors. Optical Materials Express, 2014, 4, 1770.	1.6	27
1071	Structural change and phase coexistence upon magnetic ordering in the magnetodielectric spinel Mn_3O_4 . Physical Review B, 2014, 90, .	1.1	37
1072	Microstrain in tetragonal lead-zirconate-titanate: The effect of pressure on the ionic displacements. Review of Scientific Instruments, 2014, 85, 083901.	0.6	6
1073	Recent research progress on iron- and manganese-based positive electrode materials for rechargeable sodium batteries. Science and Technology of Advanced Materials, 2014, 15, 043501.	2.8	199
1074	Magnetism-Driven Electric Polarization of Multiferroic Quasi-One-Dimensional Ca_3CoMnO_6 : First-Principles Study Using Density Functional Theory. Journal of the Physical Society of Japan, 2014, 83, 124711.	0.7	10
1075	Steric engineering of metal-halide perovskites with tunable optical band gaps. Nature Communications, 2014, 5, 5757.	5.8	787
1076	Single-Crystal Neutron Diffraction Study of Superstructure Ordering and Domain Behaviour in Brownmillerite-Type $Ca_2Fe_2O_5$. Australian Journal of Chemistry, 2014, 67, 1824.	0.5	1
1077	Discovery of the Last Remaining Binary Platinum-Group Pernitride RuN_2 . Chemistry - A European Journal, 2014, 20, 13885-13888.	1.7	57
1078	Electrokinetic detection for X-ray spectra of weakly interacting liquids: n-decane and n-nonane. Journal of Chemical Physics, 2014, 140, 234202.	1.2	7
1079	The polarization trajectory of terahertz magnetic dipole radiation in (110)-oriented $PrFeO_3$ single crystal. Journal of Applied Physics, 2014, 115, 163108.	1.1	7
1080	Piezo-antiferromagnetic effect of sawtooth-like graphene nanoribbons. Applied Physics Letters, 2014, 104, .	1.5	3
1081	Structural and ferroelectric transitions in magnetic nickelate $PbNiO_3$. New Journal of Physics, 2014, 16, 015030.	1.2	23
1082	Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites. Nature Communications, 2014, 5, 5900.	5.8	247
1083	Structural, electronic, and optical properties of $GaNO_3$: A hybrid density functional study. Journal of Applied Physics, 2014, 115, .	1.1	33
1084	Electrostatics-based finite-size corrections for first-principles point defect calculations. Physical Review B, 2014, 89, .	1.1	320
1085	Combined Computational and Experimental Study of Li Exchange Reaction at the Surface of Spinel $LiMn_2O_4$ as a Rechargeable Li-Ion Battery Cathode. Journal of Physical Chemistry C, 2014, 118, 27245-27251.	1.5	31
1086	An <i>ab initio</i> investigation of flexoelectric effect in ultrathin $BaTiO_3$ nanotubes. Journal of Applied Physics, 2014, 115, .	1.1	9

#	ARTICLE	IF	CITATIONS
1087	Electric polarization along the c-axis in the ferroelectric helimagnetic phase of $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$ ($x=0.035$). <i>Physical Review B</i> , 2014, 90, .	1.1	0
1088	Successes and failures of Hubbard-corrected density functional theory: The case of Mg doped LiCoO_2 . <i>Journal of Chemical Physics</i> , 2014, 141, 164706.	1.2	22
1089	Lone-pair interactions and photodissociation of compressed nitrogen trifluoride. <i>Journal of Chemical Physics</i> , 2014, 141, 064706.	1.2	8
1090	Hyperactive antifreeze protein from an Antarctic sea ice bacterium <i>Colwellia</i> sp. has a compound ice-binding site without repetitive sequences. <i>FEBS Journal</i> , 2014, 281, 3576-3590.	2.2	64
1091	Spin-orbit insulating state close to the cubic limit in $\text{Ca}_4\text{IrO}_{10}$. <i>Physical Review B</i> , 2014, 89, .	1.1	27
1092	Pathways towards ferroelectricity in hafnia. <i>Physical Review B</i> , 2014, 90, .	1.1	351
1093	FP-LAPW investigation of electronic, magnetic, elastic and thermal properties of Fe-doped zirconium nitride. <i>AIP Advances</i> , 2014, 4, .	0.6	7
1094	Communication: The description of strong correlation within self-consistent Green's function second-order perturbation theory. <i>Journal of Chemical Physics</i> , 2014, 140, 241101.	1.2	87
1095	Charge and orbital orderings associated with metal-insulator transition in V_6O_{13} . <i>Physical Review B</i> , 2014, 90, .	1.1	13
1096	Molecular and Polymeric Uranyl and Thorium Complexes with Sulfonate-Containing Ligands. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 58-68.	1.0	27
1097	Controlling orbital-selective Kondo effects in a single molecule through coordination chemistry. <i>Journal of Chemical Physics</i> , 2014, 141, 054702.	1.2	27
1098	First-principles predicted low-energy structures of $\text{NaSc}(\text{BH}_4)_4$. <i>Journal of Chemical Physics</i> , 2014, 140, 124708.	1.2	25
1099	First-principles study of the multimode antiferroelectric transition in PbZrO_3 . <i>Physical Review B</i> , 2014, 90, .	1.1	73
1100	Structure of Vanadium-Doped Zinc Oxide, $\text{Zn}_{1-x}\text{V}_x\text{O}$. <i>Materials and Manufacturing Processes</i> , 2014, 29, 780-788.	2.7	19
1101	Origins of hole traps in hydrogenated nanocrystalline and amorphous silicon revealed through machine learning. <i>Physical Review B</i> , 2014, 89, .	1.1	31
1103	Electron lone pair distortion facilitated metal-insulator transition in $\text{Pb}_0.33\text{V}_2\text{O}_5$ nanowires. <i>Applied Physics Letters</i> , 2014, 104, .	1.5	15
1104	Theoretical studies of Ir_5Th and Ir_5Ce nanoscale precipitates in Ir. <i>Philosophical Magazine</i> , 2014, 94, 991-1000.	0.7	2
1105	Modulation of the work function of fullerenes C_{60} and C_{70} by alkaline earth metal adsorption: A theoretical study. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2014, 32, 010601.	0.6	0

#	ARTICLE	IF	CITATIONS
1106	Ba ₄ Ga ₃ N ₃ O. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, i28-i28.	0.2	4
1107	Group IV clathrates: synthesis, optoelectronic properties, and photovoltaic applications. Proceedings of SPIE, 2014, , .	0.8	9
1108	Effect of amino ligand size of Si precursors on initial reaction with an OH-terminated Si(001) surface for atomic layer deposition. Japanese Journal of Applied Physics, 2014, 53, 08NE04.	0.8	8
1109	Transport Properties of the Layered Transition Metal Oxynictide Sr ₂ ScMPO ₃ with M=P layers (M=Mn, Ni and Tj) ETQq1 1 0.784314 rgBT3/Overlock 10 Tf 50	0.7	10
1110	Effect of Ga ³⁺ Doping on the Photoluminescence Properties of Y ₃ Al _{5-x} Ga _x O ₁₂ :Bi ³⁺ +Phosphor. ECS Journal of Solid State Science and Technology, 2014, 3, R222-R227.	0.9	33
1111	Polarization-sensitive second harmonic generation microscopy of $\hat{1}\pm$ -quartz like GeO ₂ ($\hat{1}\pm$ -GeO ₂) polycrystal. Journal Physics D: Applied Physics, 2014, 47, 455305.	1.3	4
1112	Atomic and electronic structures of YBa ₂ Cu ₃ O ₇ [001], [010] tilt and twist grain boundaries. Superconductor Science and Technology, 2014, 27, 025007.	1.8	1
1113	Effect of <i>c</i> -plane sapphire substrate miscut angle on indium content of MOVPE-grown N-polar InGaN. Japanese Journal of Applied Physics, 2014, 53, 05FL07.	0.8	7
1114	Study of New Active Materials for Rechargeable Sodium-Ion Batteries. Advances in Science and Technology, 0, , .	0.2	2
1115	Origin of the Bloch-type polarization components at the 180° domain walls in ferroelectric PbTiO ₃ . Journal of Applied Physics, 2014, 116, .	1.1	20
1116	Structure analysis of CaTi _{1-x} Sn _x O ₃ (x=0.0-1.0) solid solutions. Powder Diffraction, 2014, 29, 254-259.	0.4	5
1117	Pentalanthanum zinc diplumbide, La ₅ Zn _{1-x} Pb _{2+x} (<i>x</i> 0.6). Acta Crystallographica Section E: Structure Reports Online, 2014, 70, i2-i3.	0.2	3
1118	Integrated Approach to Structure-Based Enzymatic Drug Design: Molecular Modeling, Spectroscopy, and Experimental Bioactivity. Chemical Reviews, 2014, 114, 493-537.	23.0	100
1119	The system BaZnSn at 500 °C: Phase equilibria, crystal and electronic structure of ternary phases. Journal of Alloys and Compounds, 2014, 585, 287-298.	2.8	9
1120	The effect of chemical potential on the thermodynamic stability of carbonate ions in hydroxyapatite. Acta Biomaterialia, 2014, 10, 3716-3722.	4.1	27
1121	Insights into the adsorption of CH ₂ BrF on anatase TiO ₂ (101) surface through DFT modelling. Computational Materials Science, 2014, 81, 556-560.	1.4	4
1122	Crystal structures and ferromagnetism of Fe _x WN ₂ (x=0.74, 0.90) with defective iron triangular lattice. Journal of Alloys and Compounds, 2014, 593, 154-157.	2.8	7
1123	Comment on "Structural and Mössbauer study of the brownmillerite oxides LaSrMn _{2-x} Fe _x O ₅ (0 ≤ x ≤ 0.5)". Journal of Alloys and Compounds, 2014, 610, 212-213.	2.8	2

#	ARTICLE	IF	CITATIONS
1124	Experimental and theoretical investigations on high-pressure phase transition of Sr ₂ Fe ₂ O ₅ . <i>Physics and Chemistry of Minerals</i> , 2014, 41, 449-459.	0.3	6
1125	Phosphorus Electrodes in Sodium Cells: Small Volume Expansion by Sodiation and the Surface Stabilization Mechanism in Aprotic Solvent. <i>ChemElectroChem</i> , 2014, 1, 580-589.	1.7	196
1126	Two-dimensional metamaterials for epitaxial heterostructures. <i>Current Opinion in Solid State and Materials Science</i> , 2014, 18, 46-52.	5.6	2
1127	Study of Raman spectra for $\hat{\Gamma}^3$ -Al ₂ O ₃ models by using first-principles method. <i>Solid State Communications</i> , 2014, 178, 16-22.	0.9	60
1128	Uranyl Organic Frameworks with Polycarboxylates: Unusual Effects of a Coordinating Solvent. <i>Crystal Growth and Design</i> , 2014, 14, 1314-1323.	1.4	73
1129	Metal organic frameworks built from alkali metal ions (Li ⁺ –Cs ⁺) and 1,2,3,4-cyclobutanetetracarboxylic acid. <i>CrystEngComm</i> , 2014, 16, 1724.	1.3	12
1130	Engineered spatial inversion symmetry breaking in an oxide heterostructure built from isosymmetric room-temperature magnetically ordered components. <i>Chemical Science</i> , 2014, 5, 1599-1610.	3.7	30
1131	Structural flexibility of 4,4'-methylene diphenyl diisocyanate (4,4'-MDI): evidence from first principles calculations. <i>Journal of Molecular Modeling</i> , 2014, 20, 2097.	0.8	14
1132	Non-180° polarization rotation of ferroelectric (Bi _{0.5} Na _{0.5})TiO ₃ single crystals under electric field. <i>Physical Review B</i> , 2014, 89, .	1.1	29
1133	Synthesis and crystal structure of K ₂ NiF ₄ -type novel Gd _{1+x} Ca _{1-x} AlO ₄ N _x oxynitrides. <i>Journal of Alloys and Compounds</i> , 2014, 582, 823-826.	2.8	7
1134	Superconducting Double Perovskite Bismuth Oxide Prepared by a Low Temperature Hydrothermal Reaction. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 3599-3603.	7.2	61
1135	Highly Luminescent Colloidal Eu ³⁺ -Doped KZnF ₃ Nanoparticles for the Selective and Sensitive Detection of Cu ^{II} Ions. <i>Chemistry - A European Journal</i> , 2014, 20, 3311-3316.	1.7	51
1136	Electron density distribution and disordered crystal structure of 8H-SiAlON, Si _{3-x} Al _{1+x} O _x N _{5-x} (x~2.2). <i>Journal of Solid State Chemistry</i> , 2014, 213, 169-175.	1.4	5
1137	The compressional behaviour and the mechanical properties of talc [Mg ₃ Si ₄ O ₁₀ (OH) ₂]: a density functional theory investigation. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 639-650.	0.3	34
1138	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. <i>American Mineralogist</i> , 2014, 99, 117-127.	0.9	35
1139	New O ₂ /P ₂ -type Li-Excess Layered Manganese Oxides as Promising Multifunctional Electrode Materials for Rechargeable Li/Na Batteries. <i>Advanced Energy Materials</i> , 2014, 4, 1301453.	10.2	307
1140	Ionic Conduction in Cubic Na ₃ Ti ₃ O ₉ N, a Secondary Na-Ion Battery Cathode with Extremely Low Volume Change. <i>Chemistry of Materials</i> , 2014, 26, 3295-3305.	3.2	68
1141	Electronic structure of spinel-type LiNi _{1/2} Ge _{3/2} O ₄ and LiNi _{1/2} Mn _{3/2} O ₄ as positive electrodes for rechargeable Li-ion batteries studied by first-principles density functional theory. <i>Solid State Ionics</i> , 2014, 262, 74-76.	1.3	5

#	ARTICLE	IF	CITATIONS
1142	A Family of High-Performance Cathode Materials for Na-ion Batteries, $\text{Na}_3(\text{VO}_2)_x\text{PO}_4$ ($0 \leq x \leq 1$) (0-100%) F_{1+2x} (0-100%) O_{27} (0-100%) 24, 4603-4614.	7.8	271
1143	Depletion NO _x Made Easy by Nitrogen Doped Graphene. Catalysis Letters, 2014, 144, 1016-1022.	1.4	16
1144	Localization and Impact of Pb-Non-Bonded Electronic Pair on the Crystal and Electronic Structure of Pb ₂ YSbO ₆ . Inorganic Chemistry, 2014, 53, 5609-5618.	1.9	6
1145	Structural ground states of Cr_2		

#	ARTICLE	IF	CITATIONS
1160	Formation Principles for Vanadium Selenites: The Role of pH on Product Composition. <i>Inorganic Chemistry</i> , 2014, 53, 12027-12035.	1.9	10
1161	Long-Range Ordered Structure of Ti-B-C-N in a TiB ₂ -TiC x N ₁ Eutectic Composite. <i>Journal of the American Ceramic Society</i> , 2014, 97, 2423-2426.	1.9	13
1162	Mesoporous NaTi ₂ (PO ₄) ₃ /CMK-3 nanohybrid as anode for long-life Na-ion batteries. <i>Journal of Materials Chemistry A</i> , 2014, 2, 20659-20666.	5.2	99
1163	Research Development on Sodium-Ion Batteries. <i>Chemical Reviews</i> , 2014, 114, 11636-11682.	23.0	4,970
1164	Low Temperature Preparation and Electrochemical Properties of LiFeSi ₂ O ₆ . <i>Journal of the Electrochemical Society</i> , 2014, 161, A1642-A1647.	1.3	10
1165	Synthesis and optical band gaps of alloyed Si-Ge type II clathrates. <i>Journal of Materials Chemistry C</i> , 2014, 2, 3231-3237.	2.7	55
1166	Ab initio DFT+U analysis of oxygen transport in LaCoO ₃ : the effect of Co ³⁺ magnetic states. <i>Journal of Materials Chemistry A</i> , 2014, 2, 8060-8074.	5.2	76
1167	Efficient route to phase selective synthesis of type II silicon clathrates with low sodium occupancy. <i>CrystEngComm</i> , 2014, 16, 3940-3949.	1.3	39
1168	Structural and electronic properties of the Pt _n PAH complex (n = 1, 2) from density functional calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18586-18595.	1.3	11
1169	Structural, magnetic and theoretical calculations of a ferromagnetically coupled tetranuclear copper(ii) square complex. <i>New Journal of Chemistry</i> , 2014, 38, 1306-1314.	1.4	8
1170	(Pb,Cd)-O covalency in PbTiO ₃ -CdTiO ₃ with enhanced negative thermal expansion. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5237.	1.3	11
1171	A first principle study on Fe incorporated MTW-type zeolite. <i>Microporous and Mesoporous Materials</i> , 2014, 199, 83-92.	2.2	13
1172	Local environment dependent $\langle \text{GGA} \rangle + \langle \text{U} \rangle$ for accurate thermochemistry of transition metal compounds. <i>Physical Review B</i> , 2014, 90, .	1.1	62
1173	Electronic structure at nanocontacts of surface passivated CdSe nanorods with gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10823-10829.	1.3	5
1174	Double bubbles: a new structural motif for enhanced electron-hole separation in solids. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21098-21105.	1.3	11
1175	Covalent dependence of octahedral rotations in orthorhombic perovskite oxides. <i>Journal of Chemical Physics</i> , 2014, 141, 114704.	1.2	65
1176	Chiral one- to three-dimensional uranyl-organic assemblies from (1R,3S)-(+)-camphoric acid. <i>CrystEngComm</i> , 2014, 16, 2996.	1.3	45
1177	Fluorinated mixed valence Fe(II)-Fe(III) phosphites with channels templated by linear tetramine chains. Structural and magnetic implications of partial replacement of Fe(II) by Co(II). <i>CrystEngComm</i> , 2014, 16, 6066-6079.	1.3	3

#	ARTICLE	IF	CITATIONS
1178	A density function theory study on the NO reduction on nitrogen doped graphene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20561-20569.	1.3	53
1179	Porous Graphitic Carbon Nitride: A Possible Metal-free Photocatalyst for Water Splitting. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26479-26484.	1.5	172
1180	A new electrode material for rechargeable sodium batteries: P2-type $\text{Na}_{2/3}[\text{Mg}_{0.28}\text{Mn}_{0.72}]\text{O}_2$ with anomalously high reversible capacity. <i>Journal of Materials Chemistry A</i> , 2014, 2, 16851-16855.	5.2	284
1181	X-Ray absorption spectroscopy of LiBF_4 in propylene carbonate: a model lithium ion battery electrolyte. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23568-23575.	1.3	46
1182	Doping of rhenium disulfide monolayers: a systematic first principles study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16771-16779.	1.3	62
1183	Van der Waals density functional study of the energetics of alkali metal intercalation in graphite. <i>RSC Advances</i> , 2014, 4, 3973-3983.	1.7	145
1184	Exfoliation of one-dimensional TiO_5 chain in K_2TiO_3 . <i>Dalton Transactions</i> , 2014, 43, 13751-13755.	1.6	6
1185	Synthesis of new green-emitting $\text{KBaLa}^x\text{ScSi}_3\text{O}_9\text{:Eu}_{2+x}$ phosphors for white LEDs. <i>Optical Materials</i> , 2014, 38, 57-60.	1.7	10
1186	Novel $\text{Delta-Ta}_2\text{O}_5$ Structure Obtained from DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13652-13658.	1.5	10
1187	High oxide ion conducting solid electrolytes of bismuth and niobium co-substituted $\text{La}_2\text{Mo}_2\text{O}_9$. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 17819-17827.	3.8	21
1188	Synthesis of NASICON-type structured $\text{NaTi}_2(\text{PO}_4)_3$ "graphene nanocomposite as an anode for aqueous rechargeable Na-ion batteries. <i>Nanoscale</i> , 2014, 6, 6328-6334.	2.8	152
1189	Magnetism in Single Metalloorganic Complexes Formed by Atom Manipulation. <i>Nano Letters</i> , 2014, 14, 1196-1201.	4.5	21
1190	Gate-Opening Gas Adsorption and Host-Guest Interacting Gas Trapping Behavior of Porous Coordination Polymers under Applied AC Electric Fields. <i>Journal of the American Chemical Society</i> , 2014, 136, 12304-12313.	6.6	32
1191	Silicene on Zirconium Carbide (111). <i>Journal of Physical Chemistry C</i> , 2014, 118, 23049-23057.	1.5	129
1192	Structure of decagonal Al-Ni-Rh . <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2014, 70, 732-742.	0.5	3
1193	Investigation of the Structural Stability of Ion-Implanted $\text{Gd}_2\text{Ti}_2\text{Sn}_2\text{O}_7$ Pyrochlore-Type Oxides by Glancing Angle X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7910-7922.	1.5	16
1194	Structural phase transition and antiferromagnetic transition of Tb_3RuO_7 . <i>Journal of Solid State Chemistry</i> , 2014, 220, 22-27.	1.4	17
1195	P2-type $\text{Na}_{2/3}\text{Ni}_{1/3}\text{Mn}_{2/3}\text{Ti}_x\text{O}_2$ as a new positive electrode for higher energy Na-ion batteries. <i>Chemical Communications</i> , 2014, 50, 3677-3680.	2.2	334

#	ARTICLE	IF	CITATIONS
1196	Structural Study of the Apatite Nd ₈ Sr ₂ Si ₆ O ₂₆ by Laue Neutron Diffraction and Single-Crystal Raman Spectroscopy. <i>Inorganic Chemistry</i> , 2014, 53, 9416-9423.	1.9	7
1197	Effect of vacancies (O, Ti) on the interfacial bonding strength and magnetoelectricity in Fe/BaTiO ₃ : A first-principles study. <i>Computational Materials Science</i> , 2014, 93, 6-10.	1.4	0
1198	Phase transitions and hydrogen bonding in deuterated calcium hydroxide: High-pressure and high-temperature neutron diffraction measurements. <i>Journal of Solid State Chemistry</i> , 2014, 218, 95-102.	1.4	12
1199	Structural, transport and thermoelectric properties of Nb-doped CaLaMnO perovskite. <i>Physica B: Condensed Matter</i> , 2014, 455, 22-25.	1.3	0
1200	Structural, electronic and thermoelectric behaviour of CaMnO ₃ and CaMnO(3̂)̂. <i>Journal of Materials Chemistry A</i> , 2014, 2, 14109-14117.	5.2	98
1201	The influence of stereochemically active lone-pair electrons on crystal symmetry and twist angles in lead apatite-2<i>H</i>-type structures. <i>Mineralogical Magazine</i> , 2014, 78, 325-345.	0.6	15
1202	Uranyl Ion Complexes with all-<i>cis</i>-1,3,5-Cyclohexanetricarboxylate: Unexpected Framework and Nanotubular Assemblies. <i>Crystal Growth and Design</i> , 2014, 14, 4214-4225.	1.4	52
1203	Termination Dependence of Tetragonal CH ₃ NH ₃ Pb ₃ Surfaces for Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2903-2909.	2.1	320
1204	Increasing Complexity in the Uranyl Ionâ€™s Triacid System: From One- and Two-Dimensional Polymers to Uranylâ€™Copper(II) Dodeca- and Hexadecanuclear Species. <i>Crystal Growth and Design</i> , 2014, 14, 2665-2676.	1.4	47
1205	Dopamine Adsorption on TiO ₂ Anatase Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20688-20693.	1.5	47
1206	Effect of Offstoichiometry on the Physical Properties of Sr ₂ VO ₄ . <i>Journal of the Physical Society of Japan</i> , 2014, 83, 034708.	0.7	6
1207	Segregation and clustering of solutes at grain boundaries in Mgâ€™rare earth solid solutions. <i>Acta Materialia</i> , 2014, 79, 66-73.	3.8	185
1208	Electronically driven structural transitions in<i>A</i>₁₀(PO₄)₆F₂apatites (<i>A</i>= Ca, Sr, Pb, Cd) <i>Journal of Physical Chemistry C</i> , 2014, 70, 612-615.	0.5	11
1209	Synthesis, crystal structure and lithium ion conduction of Li ₃ BP ₂ O ₈ . <i>Dalton Transactions</i> , 2014, 43, 2294-2300.	1.6	15
1210	The crystal structure of Li ₂ B ₃ PO ₈ with the 2D-linkage of BO ₃ , BO ₄ and PO ₄ groups. <i>Dalton Transactions</i> , 2014, 43, 14525-14528.	1.6	19
1211	Structural distortion below the NÃ©el temperature in spinelGeCo ₂ O ₄ . <i>Physical Review B</i> , 2014, 90, .	1.1	26
1212	Tailored Oxygen Framework of Li ₄ Ti ₅ O ₁₂ Nanorods for High-Power Li Ion Battery. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1368-1373.	2.1	86
1213	Anisotropic strain dependence of oxygen vacancy formation in YBa ₂ Cu ₃ O _{7âˆ’} <i>Î</i>: first principle study. <i>Superconductor Science and Technology</i> , 2014, 27, 115013.	1.8	13

#	ARTICLE	IF	CITATIONS
1214	Microwave Synthesis, Photoluminescence, and Photocatalytic Activity of PVA-Functionalized Eu ³⁺ -Doped BiOX (X = Cl, Br, I) Nanoflakes. <i>Langmuir</i> , 2014, 30, 1401-1409.	1.6	138
1215	Microscopic Origins of Optical Second Harmonic Generation in Noncentrosymmetric "Nonpolar Materials. <i>Chemistry of Materials</i> , 2014, 26, 5773-5781.	3.2	74
1216	Control of Doping in Cu ₂ SnS ₃ through Defects and Alloying. <i>Chemistry of Materials</i> , 2014, 26, 4951-4959.	3.2	136
1217	Hierarchical porous metal ferrite ball-in-ball hollow spheres: General synthesis, formation mechanism, and high performance as anode materials for Li-ion batteries. <i>Nano Research</i> , 2014, 7, 1116-1127.	5.8	80
1218	Uranyl Ion Complexes with <i>trans</i> -3-(3-Pyridyl)acrylic Acid Including a Uranyl-Copper(II) Heterometallic Framework. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 4772-4778.	1.0	19
1219	Optical processes in (Y,Bi)VO ₄ doped with Eu ³⁺ or Pr ³⁺ . <i>Journal of Physics Condensed Matter</i> , 2014, 26, 405501.	0.7	12
1220	High-pressure phase transitions in FeCr ₂ O ₄ and structure analysis of new post-spinel FeCr ₂ O ₄ and Fe ₂ Cr ₂ O ₅ phases with meteoritical and petrological implications. <i>American Mineralogist</i> , 2014, 99, 1788-1797.	0.9	54
1221	First-principles study of point defects in chalcopyrite ZnSnP ₂ . <i>Physical Review B</i> , 2014, 90, .	1.1	19
1222	Hydroniumjarosite, (H ₃ O) ⁺ Fe ₃ (SO ₄) ₂ (OH) ₆ , from Cerros Pintados, Chile: Single-crystal X-ray diffraction and vibrational spectroscopic study. <i>Mineralogical Magazine</i> , 2014, 78, 535-547.	0.6	12
1223	Contributions of Correlated Acentric Atomic Displacements to the Nonlinear Second Harmonic Generation and Response. <i>ACS Photonics</i> , 2014, 1, 96-100.	3.2	25
1224	La ₃ Si ₆ N ₁₁ . <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014, 70, i23-i24.	0.2	12
1225	Field-induced spin-flop transition in a one-dimensional chain of MnV ₂ O ₆ . <i>Journal of the Korean Physical Society</i> , 2014, 64, 710-714.	0.3	5
1226	A comparative investigation on ion impact parameters and TL response of Y ₂ O ₃ :Tb ³⁺ nanophosphor exposed to swift heavy ions for space dosimetry. <i>Journal of Alloys and Compounds</i> , 2014, 589, 5-18.	2.8	34
1227	First-principles investigations of equilibrium calcium isotope fractionation between clinopyroxene and Ca-doped orthopyroxene. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 143, 132-142.	1.6	75
1228	Strong Stokes and Upconversion Luminescence from Ultrasmall Ln ³⁺ -Doped BiF ₃ (Ln=Eu ³⁺ , Yb ³⁺ /Er ³⁺) Nanoparticles Confined in a Polymer Matrix. <i>Chemistry - an Asian Journal</i> , 2014, 9, 447-451.	1.7	43
1229	The electronic structure of the antimony chalcogenide series: Prospects for optoelectronic applications. <i>Journal of Solid State Chemistry</i> , 2014, 213, 116-125.	1.4	86
1230	Space-Charge Layer Effect at Interface between Oxide Cathode and Sulfide Electrolyte in All-Solid-State Lithium-Ion Battery. <i>Chemistry of Materials</i> , 2014, 26, 4248-4255.	3.2	426
1231	Density functional theory based calculation of small-polaron mobility in hematite. <i>Physical Review B</i> , 2014, 89, .	1.1	53

#	ARTICLE	IF	CITATIONS
1232	Adsorption Process of CO ₂ on Silicalite-1 Zeolite Using Single-Crystal X-ray Method. Langmuir, 2014, 30, 3749-3753.	1.6	12
1233	Giant pressure-induced volume collapse in the pyrite mineral MnS ₂ . Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5106-5110.	3.3	37
1234	Features of the Jahn-Teller transition in Ni ^{1-x} Co _x Cr ₂ O ₄ solid solutions. Physics of the Solid State, 2014, 56, 785-791.	0.2	8
1235	Ab initio calculations of the effect of impurity iron ions on the interaction of CH ₄ and NH ₃ with nanoporous silicates. Nanotechnologies in Russia, 2014, 9, 184-188.	0.7	0
1236	Electron density distribution and disordered crystal structure of 15R-SiAlON, SiAl ₄ O ₂ N ₄ . Journal of Solid State Chemistry, 2014, 211, 124-129.	1.4	14
1237	Pressure-induced polar phases in multiferroic delafossite Cu ₂ FeO ₂ . Physical Review B, 2014, 89, ..	1.1	34
1238	Surface properties of uranium dioxide from first principles. Journal of Nuclear Materials, 2014, 452, 479-485.	1.3	10
1239	Magnetic Exchange Couplings from Noncollinear Perturbation Theory: Dinuclear Cu ^{II} Complexes. Journal of Physical Chemistry A, 2014, 118, 5841-5847.	1.1	10
1240	High-performance Flexible Broadband Photodetector Based on Organolead Halide Perovskite. Advanced Functional Materials, 2014, 24, 7373-7380.	7.8	791
1241	The hydration structure of aqueous carbonic acid from X-ray absorption spectroscopy. Chemical Physics Letters, 2014, 614, 282-286.	1.2	22
1242	Reanalysis of CO ₂ -silicalite-1 structure as monoclinic twinning. Zeitschrift Fur Kristallographie - Crystalline Materials, 2014, 229, 303-309.	0.4	9
1243	Raman study of ACu ₃ Fe ₄ O ₁₂ (A = Ca, Sr, Y and Eu). Solid State Sciences, 2014, 27, 65-68.	1.5	1
1244	Role of intermediate phase for stable cycling of Na ₇ V ₄ (P ₂ O) ₇ . Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 599-604.	3.3	136
1245	Influence of ultrasonication times on the tunable colour emission of ZnO nanophosphors for lighting applications. Ultrasonics Sonochemistry, 2014, 21, 1549-1556.	3.8	63
1246	Electronic structures of long periodic stacking order structures in Mg: A first-principles study. Journal of Alloys and Compounds, 2014, 586, 656-662.	2.8	42
1247	Structural and Photoluminescence properties of nepheline-structure NaAlSi ₃ O ₈ :Dy ³⁺ nanophosphors. Journal of Alloys and Compounds, 2014, 609, 100-106.	2.8	34
1248	Lithium diffusive behavior in Li ₂ MnO ₃ detected by muon-spin relaxation. Solid State Ionics, 2014, 262, 901-903.	1.3	11
1249	Structural stability and electronic structures of (111) twin boundaries in the rock-salt MnS. Journal of Alloys and Compounds, 2014, 582, 181-185.	2.8	20

#	ARTICLE	IF	CITATIONS
1250	Lithium ion conduction in tavorite-type LiMXO ₄ F (M ²⁺ : Al, P, Mg, S) candidate solid electrolyte materials. <i>Solid State Ionics</i> , 2014, 262, 589-592.	1.3	15
1251	Orbital-free density functional theory study of crystalline Li ⁺ -Si alloys. <i>Journal of Power Sources</i> , 2014, 254, 62-72.	4.0	18
1252	Li diffusive behavior of garnet-type oxides studied by muon-spin relaxation and QENS. <i>Solid State Ionics</i> , 2014, 262, 585-588.	1.3	27
1253	Dynamics of point defect formation, clustering and pit initiation on the pyrite surface. <i>Electrochimica Acta</i> , 2014, 127, 416-426.	2.6	52
1254	First principles investigation of the structure and electronic properties of Cu ₂ Te. <i>Computational Materials Science</i> , 2014, 81, 163-169.	1.4	32
1255	Electrochemical lithium insertion behavior of FeNbO ₄ : Structural relations and in situ conversion into FeNb ₂ O ₆ during carbon coating. <i>Materials Chemistry and Physics</i> , 2014, 145, 425-433.	2.0	41
1256	Biferroic LuCrO ₃ : Structural characterization, magnetic and dielectric properties. <i>Materials Chemistry and Physics</i> , 2014, 143, 1222-1227.	2.0	9
1257	Crystal structures of LaO _{1-x} FxBiS ₂ (x=0.23, 0.46): Effect of F doping on distortion of Bi ³⁺ -S plane. <i>Journal of Solid State Chemistry</i> , 2014, 212, 213-217.	1.4	58
1258	Epitaxial growth of indium oxyfluoride thin films by reactive pulsed laser deposition: Structural change induced by fluorine insertion into vacancy sites in bixbyite structure. <i>Thin Solid Films</i> , 2014, 559, 96-99.	0.8	3
1259	Swift heavy ion irradiation induced modification in structural, optical and luminescence properties of Y ₂ O ₃ :Tb ³⁺ nanophosphor. <i>Journal of Luminescence</i> , 2014, 146, 162-173.	1.5	62
1260	Stable sites and diffusion pathways of interstitial oxide ions in lanthanum germanate. <i>Solid State Ionics</i> , 2014, 262, 512-516.	1.3	17
1261	Electronic and atomic structures of KFe ₂ Se ₂ grain boundaries. <i>Physica C: Superconductivity and Its Applications</i> , 2014, 497, 110-118.	0.6	1
1262	Crystal structures of a pentavalent bismuthate, SrBi ₂ O ₆ and a lead bismuth oxide (Pb _{1/3} Bi _{2/3})O _{1.4} . <i>Journal of Asian Ceramic Societies</i> , 2014, 2, 150-153.	1.0	18
1263	Ferroelectric Transitions at Ferroelectric Domain Walls Found from First Principles. <i>Physical Review Letters</i> , 2014, 112, 247603.	2.9	88
1264	Dependence of the electronic and transport properties of metal-MoSe ₂ on contact structures. <i>Physical Review B</i> , 2014, 89, .	1.8	18
1265	High-throughput screening of perovskite alloys for piezoelectric performance and thermodynamic stability. <i>Physical Review B</i> , 2014, 89, .	1.1	53
1266	Predicting $\hat{\rho}^2$ precipitate morphology and evolution in Mg-RE alloys using a combination of first-principles calculations and phase-field modeling. <i>Acta Materialia</i> , 2014, 76, 259-271.	3.8	93
1267	Hubbard U calculations for gap states in dilute magnetic semiconductors. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 274202.	0.7	1

#	ARTICLE	IF	CITATIONS
1268	Prediction of structure candidates for zinc oxide as a function of pressure and investigation of their electronic properties. <i>Physical Review B</i> , 2014, 89, .	1.1	71
1269	<i>Ab initio</i> study of gallium stabilized δ -plutonium alloys and hydrogenâ€‘vacancy complexes. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 235502.	0.7	17
1270	All-In-One Light-Tunable Borated Phosphors with Chemical and Luminescence Dynamical Control Resolution. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 9160-9172.	4.0	32
1271	High-Temperature Ferrimagnetism Driven by Lattice Distortion in Double Perovskite $\text{Ca}_2\text{FeOsO}_6$. <i>Journal of the American Chemical Society</i> , 2014, 136, 3326-3329.	6.6	122
1272	Peculiarity of component interaction in Zr-Mn-Sn, Sb ternary systems. <i>Journal of Alloys and Compounds</i> , 2014, 611, 401-409.	2.8	7
1273	Investigation of uranium luminescence in SrB_4O_7 matrix by time resolved photoluminescence, thermally stimulated luminescence and electron spin resonance spectroscopy. <i>Journal of Alloys and Compounds</i> , 2014, 611, 74-81.	2.8	20
1274	Sodium-ion battery cathodes $\text{Na}_2\text{FeP}_2\text{O}_7$ and $\text{Na}_2\text{MnP}_2\text{O}_7$: diffusion behaviour for high rate performance. <i>Journal of Materials Chemistry A</i> , 2014, 2, 11807-11812.	5.2	92
1275	Swift heavy ion induced structural and luminescence characterization of Y_2O_3 : Eu^{3+} phosphor: a comparative study. <i>Luminescence</i> , 2014, 29, 480-491.	1.5	11
1276	Surface Tension Alteration on Calcite, Induced by Ion Substitution. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3078-3087.	1.5	58
1277	First-principles prediction for the stability of $\text{LiK}(\text{BH}_4)_2$. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 1539-1544.	0.7	5
1278	High-pressure synthesis, crystal structure and magnetic properties of double perovskite oxide $\text{Ba}_2\text{CuOsO}_6$. <i>Journal of Solid State Chemistry</i> , 2014, 217, 9-15.	1.4	20
1279	The effect of the sulfur on the purity and the crystallization of $\text{Cu}_2\text{ZnSnS}_4$ compound. <i>Materials Science in Semiconductor Processing</i> , 2014, 26, 583-587.	1.9	3
1280	High-temperature X-ray diffraction measurements of fluorite-related rare earth antimonates Ln_3SbO_7 ($\text{Ln}=\text{Nd, Tb}$) and their magnetic properties. <i>Journal of Solid State Chemistry</i> , 2014, 217, 16-21.	1.4	9
1281	Photocatalytic properties of lanthanide tungstates $\text{Ln}_2\text{W}_2\text{O}_9$ ($\text{Ln}=\text{La, Pr, Nd, Sm, and Gd}$). <i>Journal of Physics and Chemistry of Solids</i> , 2014, 75, 486-490.	1.9	14
1282	X-ray absorption near-edge spectroscopy study on Ge-doped $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$: enhanced ionic conductivity and defect chemistry. <i>Electrochimica Acta</i> , 2014, 115, 581-586.	2.6	33
1283	Alkali Ion Transport in Tavorite-Type ABTO_4X (A: Li, Na; B-T: Al-P, Mg-S; X: F). <i>Electrochemistry</i> , 2014, 82, 851-854.	0.6	3
1284	Electron density distribution and crystal structure of R-SiAlON , $\text{Si}_3\text{N}_x\text{Al}_6\text{O}_x$ ($\text{R}=\text{Al, O, N}$) ($x \sim 1.9$). <i>Journal of the Ceramic Society of Japan</i> , 2014, 122, 281-287.		
1285	Red-emissive Mn-doped $\text{Li}_2\text{Ge}_4\text{O}_9$ phase synthesized via glass-ceramic route. <i>Journal of the Ceramic Society of Japan</i> , 2014, 122, 725-727.	0.5	17

#	ARTICLE	IF	CITATIONS
1286	Novel Reddish Yellow-emitting Ce ³⁺ -Doped Ba ₃ Sc ₄ O ₉ Phosphors for Blue-light-based White LEDs. Chemistry Letters, 2014, 43, 828-830.	0.7	23
1287	Synthesis and Vapor-adsorption Behavior of a Flexible Porous Coordination Polymer Built from a Bis(bipyridyl)-Cu(I) Metalloligand. Chemistry Letters, 2014, 43, 1070-1072.	0.7	6
1288	Magnetic Ground State of Novel Zigzag Chain Compounds, NaCr ₂ O ₄ and Ca _{1-x} NaxCr ₂ O ₄ , Determined with Muons and Neutrons. Physics Procedia, 2015, 75, 868-875.	1.2	5
1289	Crystal structure and thermoelectric properties of the incommensurate chimney-ladder compound RhGe ₃ ($\sqrt{3} \times \sqrt{3}$ 1.293). Journal of Materials Research, 2015, 30, 2611-2617.	1.2	12
1290	Electro-vibrational coupling effects on intrinsic friction in transition metal dichalcogenides. RSC Advances, 2015, 5, 106809-106818.	1.7	15
1291	Enhanced thermoelectric performance of amorphous Nb based oxynitrides. Physica B: Condensed Matter, 2015, 479, 96-100.	1.3	10
1292	Luminescence Properties of New Blue-Emitting Sialon Polytypoid Phosphor. ECS Journal of Solid State Science and Technology, 2015, 4, R114-R117.	0.9	9
1293	Anion-Anion Bonding and Topology in Ternary Iridium Seleno-Stannides. Inorganic Chemistry, 2015, 54, 11993-12001.	1.9	5
1294	Theory of Hydrogen Migration in Organic-Inorganic Halide Perovskites. Angewandte Chemie, 2015, 127, 12614-12618.	1.6	8
1296	Novel green-emitting Ho ³⁺ -doped scandate phosphors. Journal of the Ceramic Society of Japan, 2015, 123, 880-883.	0.5	5
1298	First-Principles Materials Design of High-Performing Bulk Photovoltaics with the NbLi_3O_3 . Physical Review Applied, 2015, 4, 041101.	1.5	30
1299	Variation of magnetic ground state of SrCr_2O_7 . Physical Review Applied, 2015, 4, 041102.	1.5	43
1300	Raman study of magnetic excitations and magnetoelastic coupling in SrCr_2O_7 . Physical Review B, 2015, 91, .	1.1	12
1301	Variation of magnetic ground state of SrCr_2O_7 and SrCr_2O_4 . Physical Review B, 2015, 91, .	1.1	12
1302	Anharmonicity and phase stability of antiperovskite Li_3OCl . Physical Review B, 2015, 91, .	1.1	47
1303	Effect of disorder on the dilute equilibrium vacancy concentrations of multicomponent crystalline solids. Physical Review B, 2015, 91, .	1.1	17
1304	Ferroelectricity from coupled cooperative Jahn-Teller distortions and octahedral rotations in ordered Ruddlesden-Popper manganates. Physical Review B, 2015, 92, .	1.1	23
1305	Li-ion diffusion in Li_4O_{12} and LiTi_2O_4 . Physical Review B, 2015, 92, .	1.1	55

#	ARTICLE	IF	CITATIONS
1306	First-principles calculation of charged capacitors under open-circuit conditions using the orbital-separation approach. Physical Review B, 2015, 92, . Deep recombination centers in smml:math	1.1	2
1307	$C_{u_2ZnSnS_4}$ revealed by screened-exchange hybrid density functional theory. Physical Review B, 2015, 92, .	1.1	34
1308	New class of planar ferroelectric Mott insulators via first-principles design. Physical Review B, 2015, 92, .	1.1	4
1309	Piezomagnetolectric Effect of Spin Origin in Dysprosium Orthoferrite. Physical Review Letters, 2015, 115, 197205.	2.9	19
1310	Two kinds of in-plane resistivity anisotropy in $Fe_{1-x}Te$ ($x=0.09$) as seen via synchrotron radiation x-ray diffraction and in situ resistivity measurements. Physical Review B, 2015, 91, .	1.1	5
1311	Computational Study on Thermal Spin-Crossover Behavior for Coordination Polymers Possessing $[Fe(NCS)_2(pyridine)_4]$ Unit. Bulletin of the Chemical Society of Japan, 2015, 88, 1164-1170.	2.0	10
1312	Energy levels scheme simulation of divalent cobalt doped bismuth germanate. AIP Conference Proceedings, 2015, . .	0.3	0
1313	The electronic properties of impurities (N, C, F, Cl and S) in Ag_3PO_4 : A hybrid functional method study. Scientific Reports, 2015, 5, 12750.	1.6	6
1314	Study of σ_3 $BaZrO_3$ (210)[001] tilt grain boundaries using density functional theory and a space charge layer model. Journal of the Ceramic Society of Japan, 2015, 123, 245-249.	0.5	9
1315	In-plane chemical pressure essential for superconductivity in BiCh ₂ -based (Ch: S, Se) layered structure. Scientific Reports, 2015, 5, 14968.	1.6	104
1316	Materials Prediction via Classification Learning. Scientific Reports, 2015, 5, 13285.	1.6	68
1317	Crystal structure and electron density distribution of $La_{1.9}Bi_{0.1}Mo_2O_9$ fast oxide ion conductor. AIP Conference Proceedings, 2015, . .	0.3	0
1318	Growth and characterization of $R(O,F)BiS_2$ (R = La, Ce, Pr, Nd) superconducting single crystals. Novel Superconducting Materials, 2015, 1, .	0.8	18
1319	Magnetic Phases in $Sr_{1-x}Ca_xCo_2P_2$ Studied by ^{57}Fe SR. Physics Procedia, 2015, 75, 426-434.	1.2	1
1320	High-temperature stability of Y_2O_3 -ZrO ₂ . Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 292-298.	0.7	21
1321	Second-sphere Complexation of Thorium(IV) by Cucurbit[6]uril with Included Perrhenate Counterions: Crystal Structure and Hirshfeld Surface Analysis. European Journal of Inorganic Chemistry, 2015, 2015, 2037-2040.	1.0	8
1322	Atomistic simulation of defected magnesium hydroxide as flame retardants. Transactions of Nonferrous Metals Society of China, 2015, 25, 4080-4088.	1.7	10
1323	Hybrid Organic-Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	11.1	372

#	ARTICLE	IF	CITATIONS
1324	Time- and Energy-Efficient Solution Combustion Synthesis of Binary Metal Tungstate Nanoparticles with Enhanced Photocatalytic Activity. <i>ChemSusChem</i> , 2015, 8, 1652-1663.	3.6	44
1325	Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases. <i>New Journal of Physics</i> , 2015, 17, 093004.	1.2	15
1326	From Bonding Asymmetry to Anharmonic Rattling in $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ Tetrahedrites: When Lone-Pair Electrons Are Not So Lonely. <i>Advanced Functional Materials</i> , 2015, 25, 3648-3657.	7.8	177
1327	Theory of Hydrogen Migration in Organic-Inorganic Halide Perovskites. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12437-12441.	7.2	134
1328	Synthesis and Characterisation of $\text{Li}_{1-x}\text{Na}_x\text{Ni}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ as Cathode Materials for Rechargeable Lithium Batteries. <i>Materials Science Forum</i> , 2015, 819, 232-237.	0.3	0
1329	Hazardous Doping for Photo-Electrochemical Conversion: The Case of Nb-Doped Fe_2O_3 from First Principles. <i>Molecules</i> , 2015, 20, 19900-19906.	1.7	27
1331	High-Speed Deposition of Highly-Oriented Calcium Titanate Film by Laser CVD. <i>Funtai Oyobi Fummatsu Yakin/Journal of the Japan Society of Powder and Powder Metallurgy</i> , 2015, 63, 123-127.	0.1	5
1332	Ab initio Studies of O_2 Adsorption on (110) Nickel-Rich Pentlandite ($\text{Fe}_4\text{Ni}_5\text{S}_8$) Mineral Surface. <i>Minerals (Basel, Switzerland)</i> , 2015, 5, 665-678.	0.8	23
1333	Benchmark study of the Mössbauer isomer shifts of Eu and Np complexes by relativistic DFT calculations for understanding the bonding nature of f-block compounds. <i>Dalton Transactions</i> , 2015, 44, 8080-8088.	1.6	24
1334	Facet-dependent photocatalytic and antibacterial properties of Ag_2WO_4 crystals: combining experimental data and theoretical insights. <i>Catalysis Science and Technology</i> , 2015, 5, 4091-4107.	2.1	123
1335	Platinum-Doped Fe_2O_3 for Enhanced Water Splitting Efficiency: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5836-5847.	1.5	73
1336	Hydrothermal synthesis and crystal structure analysis of two new cadmium bismuthates, CdBi_2O_6 and $\text{Cd}_{0.37}\text{Bi}_{0.63}\text{O}_{1.79}$. <i>Journal of Asian Ceramic Societies</i> , 2015, 3, 251-254.	1.0	18
1337	Temperature dependent electron paramagnetic resonance (EPR) of SrZrO . <i>Journal of Magnetism and Magnetic Materials</i> , 2015, 391, 101-107.	1.0	14
1338	Spin rotation driven ferroelectric polarization with a 180° flop in double-perovskite $\text{Lu}_2\text{CoMnO}_6$. <i>RSC Advances</i> , 2015, 5, 43432-43439.	1.7	8
1339	Anisotropy in the Raman scattering of a $\text{CaFeO}_{2.5}$ single crystal and its link with oxygen ordering in Brownmillerite frameworks. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 225403.	0.7	19
1340	Informatics-Aided Density Functional Theory Study on the Li Ion Transport of Tavorite-Type LiMTO_4F ($\text{M}^{3+} = \text{T}^{5+}$, $\text{M}^{2+} = \text{T}^{6+}$). <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1158-1168.	2.5	42
1341	Modulating the magnetic behavior of $\text{Fe}(\text{MOF-74})$ by the high electron affinity of the guest molecule. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16977-16982.	1.3	23
1342	Theoretical investigations of novel zinc oxide polytypes and in-depth study of their electronic properties. <i>RSC Advances</i> , 2015, 5, 25929-25935.	1.7	28

#	ARTICLE	IF	CITATIONS
1343	Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion. <i>Journal of Materials Science</i> , 2015, 50, 5715-5722.	1.7	8
1344	Synthesis of Na ₂ Mg ₃ X ₂ (X = Sn, Pb) and Na ₄ Mg ₄ Sn ₃ and their crystal structures and thermoelectric properties. <i>Japanese Journal of Applied Physics</i> , 2015, 54, 07JC04.	0.8	2
1345	Structures, electronic properties and stability phase diagrams for copper(II) bromide surfaces. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9341-9351.	1.3	14
1346	Tailoring Nanoscale Friction in MX ₂ Transition Metal Dichalcogenides. <i>Inorganic Chemistry</i> , 2015, 54, 5739-5744.	1.9	40
1347	High-performance transition metal-doped Pt ₃ Ni octahedra for oxygen reduction reaction. <i>Science</i> , 2015, 348, 1230-1234.	6.0	1,623
1348	Interfacial Effects in μ -Li _x VOPO ₄ and Evolution of the Electronic Structure. <i>Chemistry of Materials</i> , 2015, 27, 8211-8219.	3.2	37
1349	Structural and electronic properties of alkali metal peroxides at high pressures. <i>RSC Advances</i> , 2015, 5, 104337-104342.	1.7	12
1350	Synthesis, Direct Formation under High Pressure, Structure, and Electronic Properties of LiNbO ₃ -type Oxide PbZnO ₃ . <i>Inorganic Chemistry</i> , 2015, 54, 11405-11410.	1.9	31
1351	Assessing the Bonding Properties of Individual Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12862-12867.	1.1	14
1352	Identifying and rationalizing the morphological, structural, and optical properties of $\text{I}^2\text{-Ag}_2\text{MoO}_4$ microcrystals, and the formation process of Ag nanoparticles on their surfaces: combining experimental data and first-principles calculations. <i>Science and Technology of Advanced Materials</i> , 2015, 16, 065002.	2.8	61
1353	Improved conductivity of NdFeO ₃ through partial substitution of Nd by Ca: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29097-29102.	1.3	9
1354	Quantifying electronic correlation strength in a complex oxide: A combined DMFT and ARPES study of LaNiO_3 . <i>Physical Review B</i> , 2015, 92, ...	1.1	32
1355	Predicting complex mineral structures using genetic algorithms. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 425201.	0.7	3
1356	Atomic and electronic structures of Si(1 1) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 227 Td (1)- $\sqrt{3}$ and (6 \AA - 6)-Au surfaces. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 475001.	0.7	3
1357	Covalent effects in magnetic ferroelectrics Mn ₃ (M _{1-x} M ₂) ₃ (M ₁ = Ti, Sn). <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 626-634.	0.7	8
1358	Excitation spectra and luminescence decay analysis of K ⁺ compensated Dy ³⁺ doped CaMoO ₄ phosphors. <i>RSC Advances</i> , 2015, 5, 7380-7387.	1.7	121
1359	The effect of in-plane strain on the electronic properties of LaAlO ₃ /SrTiO ₃ interface. <i>Computational Materials Science</i> , 2015, 99, 57-61.	1.4	16
1360	Domain boundaries and their influence on Li migration in solid-state electrolyte (La,Li)TiO ₃ . <i>Journal of Power Sources</i> , 2015, 276, 203-207.	4.0	75

#	ARTICLE	IF	CITATIONS
1361	High-pressure high-temperature transitions in MgCr ₂ O ₄ and crystal structures of new Mg ₂ Cr ₂ O ₅ and post-spinel MgCr ₂ O ₄ phases with implications for ultrahigh-pressure chromitites in ophiolites. <i>American Mineralogist</i> , 2015, 100, 59-65.	0.9	43
1362	Impact of W on structural evolution and diffusivity of Ni-W melts: an ab initio molecular dynamics study. <i>Journal of Materials Science</i> , 2015, 50, 1071-1081.	1.7	11
1363	Atomic insight into electrochemical inactivity of lithium chromate (LiCrO ₂): Irreversible migration of chromium into lithium layers in surface regions. <i>Journal of Power Sources</i> , 2015, 273, 1218-1225.	4.0	45
1364	Synergistic Oxygen Evolving Activity of a TiO ₂ -Rich Reconstructed SrTiO ₃ (001) Surface. <i>Journal of the American Chemical Society</i> , 2015, 137, 2939-2947.	6.6	58
1365	Exploring the possibilities of two-dimensional transition metal carbides as anode materials for sodium batteries. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5000-5005.	1.3	159
1366	Theoretical limits on the stability of single-phase kesterite-Cu ₂ ZnSnS ₄ . <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	22
1367	Fully Electron-Transferred Donor/Acceptor Layered Frameworks with TCNQ ²⁻ . <i>Inorganic Chemistry</i> , 2015, 54, 1518-1527.	1.9	33
1368	Growth history and textures of quartz twinned in accordance with the Japan law. <i>European Journal of Mineralogy</i> , 2015, 27, 71-80.	0.4	4
1369	Strain effects on the electronic structure of ZnSnP ₂ via modified Becke-Johnson exchange potential. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 427-430.	0.9	9
1370	First principles studies of GeTe based dilute magnetic semiconductors. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 015501.	0.7	17
1371	Role of Noncovalent Interactions in Vanadium Tellurite Chain Connectivities. <i>Inorganic Chemistry</i> , 2015, 54, 694-703.	1.9	14
1372	First-principles studies of lone-pair-induced distortions in epitaxial phases of perovskite SnTiO_3 and PbTiO_3 . <i>Physical Review B</i> , 2015, 91, .	1.1	29
1373	Uranyl and Uranyl ³⁺ Block Cation Complexes with 1,3-Adamantanedicarboxylate: Crystal Structures, Luminescence, and Magnetic Properties. <i>Inorganic Chemistry</i> , 2015, 54, 2838-2850.	1.9	63
1374	High-Pressure Synthesis, Crystal Structures, and Magnetic Properties of 5d Double-Perovskite Oxides Ca ₂ MgOsO ₆ and Sr ₂ MgOsO ₆ . <i>Inorganic Chemistry</i> , 2015, 54, 3422-3431.	1.9	61
1375	A new n-type half-Heusler thermoelectric material NbCoSb. <i>Materials Research Bulletin</i> , 2015, 70, 773-778.	2.7	89
1376	Structural refinement, Raman spectroscopy, optical and electrical properties of (Ba ^x Sr _{1-x})MoO ₄ ceramics. <i>Journal of Materials Science: Materials in Electronics</i> , 2015, 26, 8319-8335.	1.1	30
1377	Quantifying the origin of inter-adsorbate interactions on reactive surfaces for catalyst screening and design. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22227-22234.	1.3	2
1378	Structural Variations in the Uranyl/4,4'-Biphenyldicarboxylate System. Rare Examples of 2D \rightarrow 3D Polycatenated Uranyl ²⁺ Organic Networks. <i>Inorganic Chemistry</i> , 2015, 54, 8093-8102.	1.9	73

#	ARTICLE	IF	CITATIONS
1379	Atomsk: A tool for manipulating and converting atomic data files. <i>Computer Physics Communications</i> , 2015, 197, 212-219.	3.0	1,021
1380	Atomic oxygen adsorption on 3.125 at.% Ga stabilized $\hat{\Gamma}$ -Pu (1 1 1) surface. <i>Journal of Alloys and Compounds</i> , 2015, 643, 253-262.	2.8	14
1381	Synthesis and crystal structure of Ba ₂ B ₁₂ Si ₅ N ₂₇ containing [Si ₂] dumbbells. <i>Journal of Solid State Chemistry</i> , 2015, 230, 390-396.	1.4	7
1382	Guided design of copper oxysulfide superconductors. <i>Europhysics Letters</i> , 2015, 111, 17002.	0.7	8
1383	Sc ₂ NiMnO ₆ : A Double-Perovskite with a Magnetodielectric Response Driven by Multiple Magnetic Orders. <i>Inorganic Chemistry</i> , 2015, 54, 8012-8021.	1.9	35
1384	Three-dimensionally ordered porous TiNb ₂ O ₇ nanotubes: a superior anode material for next generation hybrid supercapacitors. <i>Journal of Materials Chemistry A</i> , 2015, 3, 16785-16790.	5.2	96
1385	Morphology and Active-Site Engineering for Stable Round-Trip Efficiency Li ⁺ O ₂ Batteries: A Search for the Most Active Catalytic Site in Co ₃ O ₄ . <i>ACS Catalysis</i> , 2015, 5, 5116-5122.	5.5	99
1386	Effects of Ag-embedding on electronic and ionic conductivities of LiMnPO ₄ and its performance as a cathode for lithium-ion batteries. <i>Nanoscale</i> , 2015, 7, 13860-13867.	2.8	21
1387	Optical processes in YVO ₄ :Eu ³⁺ across zircon-to-scheelite phase transition. <i>Journal of Luminescence</i> , 2015, 165, 19-22.	1.5	8
1388	Anomalous structural dynamics in liquid Al ₈₀ Cu ₂₀ : An ab initio molecular dynamics study. <i>Acta Materialia</i> , 2015, 97, 75-85.	3.8	62
1389	Rational Design of Pt ₃ Ni Surface Structures for the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17735-17747.	1.5	44
1390	Long- and short-range structure studies of KBT-KBZ solid-solutions using synchrotron radiation. <i>Dalton Transactions</i> , 2015, 44, 10681-10688.	1.6	11
1391	First-principles calculations of divalent substitution of Ca ²⁺ in tricalcium phosphates. <i>Acta Biomaterialia</i> , 2015, 23, 329-337.	4.1	58
1392	Two-dimensional assemblies in f-element ion (UO ₂ ²⁺ , Yb ³⁺) complexes with two cyclohexyl-based polycarboxylates. <i>Polyhedron</i> , 2015, 98, 5-11.	1.0	20
1393	High thermal stability of red emission in Mn-doped benitoite-type strontium silicogermanate. <i>Applied Physics Express</i> , 2015, 8, 072603.	1.1	8
1394	Straightforward understanding of the structures of metastable $\hat{\Gamma}$ - $\hat{\Gamma}$ ³ and possible ordered phases in uranium-niobium alloys from crystallographic simulation. <i>Journal of Alloys and Compounds</i> , 2015, 648, 389-396.	2.8	7
1395	Bonding Study on the Chemical Separation of Am(III) from Eu(III) by S-, N-, and O-Donor Ligands by Means of All-Electron ZORA-DFT Calculation. <i>Inorganic Chemistry</i> , 2015, 54, 7103-7109.	1.9	45
1396	Jahn-Teller effect in 4T _{2g} excited state of Mn ²⁺ :MgO. <i>Chemical Physics</i> , 2015, 460, 26-30.	0.9	3

#	ARTICLE	IF	CITATIONS
1397	Uranyl Ion Complexes with 1,1'-Biphenyl-2,2',6,6'-tetracarboxylic Acid: Structural and Spectroscopic Studies of One- to Three-Dimensional Assemblies. <i>Inorganic Chemistry</i> , 2015, 54, 6296-6305.	1.9	36
1398	Nano-sized Superlattice Clusters Created by Oxygen Ordering in Mechanically Alloyed Fe Alloys. <i>Scientific Reports</i> , 2015, 5, 11772.	1.6	11
1399	Structural phase transitions and magnetic and spectroscopic properties of the double perovskites $\text{Sr}_2\text{Co}_{1-x}\text{Mg}_x\text{TeO}_6$ ($x = 0.1, 0.2$ and 0.5). <i>Dalton Transactions</i> , 2015, 44, 13716-13734.	1.6	14
1400	Optoelectronic properties and polar nano-domain behavior of sol-gel derived $\text{K}_{0.5}\text{Na}_{0.5}\text{Nb}_{1-x}\text{Mn}_x\text{O}_3$ nanocrystalline films with enhanced ferroelectricity. <i>Journal of Materials Chemistry C</i> , 2015, 3, 8225-8234.	2.7	33
1401	Benzimidazole-functionalized ancillary ligands for heteroleptic $\text{Ru}(\text{II})$ complexes: synthesis, characterization and dye-sensitized solar cell applications. <i>Dalton Transactions</i> , 2015, 44, 14697-14706.	1.6	26
1402	Intense NIR emissions at $0.8 \mu\text{m}$, $1.47 \mu\text{m}$, and $1.53 \mu\text{m}$ from colloidal $\text{LiYbF}_4\text{:Ln}^{3+}$ ($\text{Ln} = \text{Tm, Er, Nd, Sm}$). <i>Journal of Solid State Chemistry</i> , 2015, 229, 17577-17583.	1.3	11
1403	Synthesis, crystal structure and photoluminescence of $(\text{Ba}_{0.99}\text{Eu}_{0.01})\text{Al}_3\text{Si}_4\text{N}_9$. <i>Journal of Solid State Chemistry</i> , 2015, 228, 258-265.	1.4	3
1404	Octahedral and trigonal-prismatic coordination preferences in Nb-, Mo-, Ta-, and W-based ABX_2 layered oxides, oxynitrides, and nitrides. <i>Journal of Solid State Chemistry</i> , 2015, 229, 272-277.	1.4	17
1405	Synthesis of Eu^{3+} -activated BaMoO_4 phosphors and their Judd-Ofelt analysis: Applications in lasers and white LEDs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 141-148.	2.0	60
1406	Photoelectrochemical epitaxy of silver oxide clathrate $\text{Ag}_7\text{O}_8\text{M}$ ($\text{M} = \text{Cu, Ni, Zn}$). <i>CrystEngComm</i> , 2015, 17, 3701-3707.	1.3	8
1407	Modular design of SPIRO-OMeTAD analogues as hole transport materials in solar cells. <i>Chemical Communications</i> , 2015, 51, 8935-8938.	2.2	64
1408	Eu^{3+} -activated SrMoO_4 phosphors for white LEDs applications: Synthesis and structural characterization. <i>Optical Materials</i> , 2015, 42, 178-186.	1.7	71
1409	Hydrothermal synthesis of a new Bi-based $(\text{Ba}_{0.82}\text{K}_{0.18})(\text{Bi}_{0.53}\text{Pb}_{0.47})\text{O}_3$ superconductor. <i>Journal of Alloys and Compounds</i> , 2015, 634, 208-214.	2.8	38
1410	Crystal structure and thermal expansion of a CsCe_2Cl_7 scintillator. <i>Journal of Solid State Chemistry</i> , 2015, 227, 142-149.	1.4	6
1411	Structural variations in terbium(III) complexes with 1,3-adamantanedicarboxylate and diverse co-ligands. <i>Journal of Solid State Chemistry</i> , 2015, 227, 265-272.	1.4	9
1412	An investigation of the thermal stability of Nd Y ZrO_2 inert matrix fuel materials. <i>Journal of Alloys and Compounds</i> , 2015, 635, 245-255.	2.8	8
1413	Ferroelectricity induced by ferriaxial crystal rotation and spin helicity in B_2O_3 -site-ordered double-perovskite multiferroic InMn_2O_7 . <i>Nature Communications</i> , 2015, 6, 7971.	1.1	17
1414	Magnetic ordering and ferroelectricity in multiferroic AgFeO_2 . <i>Physical Review B</i> , 2015, 91, 014407.	1.1	18

#	ARTICLE	IF	CITATIONS
1415	Structural, vibrational and thermophysical properties of pyrophyllite by semi-empirical density functional modelling. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 609-627.	0.3	27
1416	Signature of antiferromagnetism in entropy maximized charge density distribution of melt grown diluted magnetic semiconductor $\text{Ge}_{1-x}\text{V}_x$. <i>Journal of Materials Science: Materials in Electronics</i> , 2015, 26, 3772-3780.	1.1	0
1417	Incorporation of Mg^{2+} in surface Ca^{2+} sites of aragonite: an ab initio study. <i>Progress in Earth and Planetary Science</i> , 2015, 2, .	1.1	14
1418	Solvent effects in solvo-hydrothermal synthesis of uranyl ion complexes with 1,3-adamantanediacetate. <i>CrystEngComm</i> , 2015, 17, 4006-4018.	1.3	32
1419	Structures and magnetic properties of rare earth double perovskites containing antimony or bismuth Ba_2LnMO_6 (Ln=rare earths; M=Sb, Bi). <i>Journal of Solid State Chemistry</i> , 2015, 227, 132-141.	1.4	18
1420	Spectral and CIE parameters of red emitting $\text{Gd}_3\text{Ga}_5\text{O}_{12}:\text{Eu}^{3+}$ phosphor. <i>Journal of Luminescence</i> , 2015, 159, 317-324.	1.5	45
1421	Band engineering of $\text{AgSb}_{1-x}\text{Bi}_x\text{O}_3$ for photocatalytic water oxidation under visible light. <i>Journal of Materials Chemistry A</i> , 2015, 3, 8466-8474.	5.2	18
1422	Photoluminescence and photocatalytic activity of monodispersed colloidal ligand free Ln^{3+} -doped PbMoO_4 nanocrystals. <i>RSC Advances</i> , 2015, 5, 45611-45617.	1.7	15
1423	Joint Experimental and Computational ^{17}O and ^1H Solid State NMR Study of $\text{Ba}_2\text{Ln}_2\text{O}_4(\text{OH})_2$ Structure and Dynamics. <i>Chemistry of Materials</i> , 2015, 27, 3861-3873.	3.2	27
1424	Tuning the ferroelectric polarization in AA^2MnWO_6 double perovskites through A cation substitution. <i>Dalton Transactions</i> , 2015, 44, 10644-10653.	1.6	29
1425	Spin reorientation transition process in single crystal NdFeO_3 . <i>Solid State Communications</i> , 2015, 211, 47-51.	0.9	41
1426	Ultralong $\text{SrLi}_2\text{Ti}_6\text{O}_{14}$ nanowires composed of single-crystalline nanoparticles: Promising candidates for high-power lithium ions batteries. <i>Nano Energy</i> , 2015, 13, 18-27.	8.2	79
1427	EELS study of Fe- or Co-doped titania nanosheets. <i>Microscopy (Oxford, England)</i> , 2015, 64, 77-85.	0.7	4
1428	Single Molecule Investigation of Glycine-Chlorite Interaction by Cross-Correlated Scanning Probe Microscopy and Quantum Mechanics Simulations. <i>Langmuir</i> , 2015, 31, 4453-4463.	1.6	21
1429	Proton conduction at BaO-terminated (001) BaZrO_3 surface using density functional theory. <i>Solid State Ionics</i> , 2015, 275, 19-22.	1.3	25
1430	Structure of superhard tungsten tetraboride: A missing link between MB_2 and MB_{12} higher borides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 3223-3228.	3.3	82
1431	A combined single crystal neutron/X-ray diffraction and solid-state nuclear magnetic resonance study of the hybrid perovskites $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X = I, Br and Cl). <i>Journal of Materials Chemistry A</i> , 2015, 3, 9298-9307.	5.2	253
1432	Effects of Gallium Doping in Garnet-Type $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolytes. <i>Chemistry of Materials</i> , 2015, 27, 2821-2831.	3.2	120

#	ARTICLE	IF	CITATIONS
1433	Hydride ion formation in stoichiometric UO_2 . <i>Chemical Communications</i> , 2015, 51, 16209-16212.	2.2	17
1434	Electron-Transferred Donor/Acceptor Ferrimagnet with $T_C = 91$ K in a Layered Assembly of Paddlewheel $[\text{Ru}_2]$ Units and TCNQ. <i>Inorganic Chemistry</i> , 2015, 54, 10001-10006.	1.9	27
1435	Photocatalytic splitting of water on s-triazine based graphitic carbon nitride: an ab initio investigation. <i>Journal of Materials Chemistry A</i> , 2015, 3, 23011-23016.	5.2	53
1436	Pressure-induced transformation processes in ferroelastic $\text{Pb}_3(\text{P} \llcorner \text{Tj ETQq1 1 0.784314 rgBT /Overloc$ Kristallographie - Crystalline Materials, 2015, 230, 593-603.	0.4	4
1437	Compound semiconductor alloys: From atomic-scale structure to bandgap bowing. <i>Applied Physics Reviews</i> , 2015, 2, .	5.5	50
1438	A study of the electronic structure and structural stability of $\text{Gd}_2\text{Ti}_2\text{O}_7$ based glass-ceramic composites. <i>RSC Advances</i> , 2015, 5, 80939-80949.	1.7	18
1439	Vibrational Properties of the Organic-Inorganic Halide Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ from Theory and Experiment: Factor Group Analysis, First-Principles Calculations, and Low-Temperature Infrared Spectra. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25703-25718.	1.5	276
1440	Comparison and analysis of Eu^{3+} luminescence in $\text{Y}_3\text{Al}_5\text{O}_{12}$ and $\text{Y}_3\text{Ga}_5\text{O}_{12}$ hosts material for red lighting phosphor. <i>Materials Chemistry and Physics</i> , 2015, 166, 167-175.	2.0	33
1441	Crystal Structures and Magnetic Properties of Nickel Chain Compounds $\text{PbM}_2\text{Ni}_6\text{Te}_3\text{O}_{18}$ (M = Mn, Cd). <i>Inorganic Chemistry</i> , 2015, 54, 10725-10731.	1.9	8
1442	Factors Contributing to Path Hysteresis of Displacement and Conversion Reactions in Li Ion Batteries. <i>Chemistry of Materials</i> , 2015, 27, 7593-7600.	3.2	27
1443	Two-Dimensional Transition Metal Dichalcogenide Monolayers as Promising Sodium Ion Battery Anodes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26374-26380.	1.5	279
1444	The structure of H_2TiO_3 a short discussion on Lithium recovery from salt lake brine by H_2TiO_3 . <i>Dalton Transactions</i> , 2015, 44, 15721-15724.	1.6	23
1445	Solid-Solution Hardening in Mg-Gd-TM (TM = Ag, Zn, and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study. <i>Jom</i> , 2015, 67, 2433-2441.	0.9	17
1446	Single crystal growth and characterization of kagomé-lattice shandites $\text{Co}_3\text{Sn}_2\text{In}_2$. <i>Journal of Crystal Growth</i> , 2015, 426, 208-213.	0.7	43
1447	Elucidating the origins of phase transformation hysteresis during electrochemical cycling of $\text{Li} \llcorner \text{Sb}$ electrodes. <i>Journal of Materials Chemistry A</i> , 2015, 3, 18928-18943.	5.2	48
1448	GW Band Structures and Carrier Effective Masses of $\text{CH}_3\text{NH}_3\text{PbI}_3$ and Hypothetical Perovskites of the Type APbI_3 : A = NH_4 , PH_4 , AsH_4 , and SbH_4 . <i>Journal of Physical Chemistry C</i> , 2015, 119, 25209-25219.	1.5	144
1449	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe_2Br_7 . <i>Journal of Materials Chemistry C</i> , 2015, 3, 11366-11376.	2.7	14
1450	Periodic model of an LTA framework. <i>Journal of Molecular Modeling</i> , 2015, 21, 275.	0.8	5

#	ARTICLE	IF	CITATIONS
1451	Theoretical description of efficiency enhancement in DSSCs sensitized by newly synthesized heteroleptic Ru complexes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29574-29585.	1.3	20
1452	Structural and magnetic studies on Fe doped zinc oxide, $Zn_{1-x}Fe_xO$ synthesized by solid state reaction. <i>Journal of Materials Science: Materials in Electronics</i> , 2015, 26, 9882-9890.	1.1	1
1453	Insights into the Lithium-Ion Conduction Mechanism of Garnet-Type Cubic $Li_5La_3Ta_2O_{12}$ by ab-Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20783-20791.	1.5	25
1454	Correlation of structure and ion conduction in $La_{2-x}Y_xMo_2O_9$ ($0 \leq x \leq 0.2$) oxygen ion conductors. <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	12
1455	Structure and electrochemical detection of xenobiotic micro-pollutant hydroquinone using CeO_2 nanocrystals. <i>RSC Advances</i> , 2015, 5, 70558-70565.	1.7	11
1456	$AgPO_2F_2$ and $Ag_9(PO_2F_2)_{14}$: the first $Ag(i)$ and $Ag(ii)$ difluorophosphates with complex crystal structures. <i>Dalton Transactions</i> , 2015, 44, 19478-19486.	1.6	8
1457	Understanding oxygen adsorption on 9.375 at. % Ga-stabilized $\hat{\Gamma}$ -Pu (111) surface: A DFT study. <i>Journal of Alloys and Compounds</i> , 2015, 653, 411-421.	2.8	7
1458	Investigation of interfaces in Mg/Nb multilayer thin films. <i>Computational Materials Science</i> , 2015, 108, 212-225.	1.4	10
1459	Image definition evaluation functions for X-ray crystallography: a new perspective on the phase problem. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2015, 71, 526-533.	0.0	2
1460	Field emission characteristics of pristine and lithium-doped boron nanotubes: A theoretical study. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , 2015, 33, 050602.	0.6	1
1461	Synthesis and Crystal Structures of $BaLaSi_2$ with cis-trans Si Chains and Ba_5LaSi_6 with Pentagonal Si Rings. <i>Inorganic Chemistry</i> , 2015, 54, 9188-9194.	1.9	2
1462	Magnetic ordering and electronic structure of the ternary iron arsenide $BaFe_2As_2$. <i>International Journal of Modern Physics B</i> , 2015, 29, 1550182.	1.0	0
1463	Can we judge an oxide by its cover? The case of platinum over $\hat{\Gamma}$ - Fe_2O_3 from first principles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24129-24137.	1.3	24
1464	Probing the effect of radiation damage on the structure of rare-earth phosphates. <i>Journal of Alloys and Compounds</i> , 2015, 653, 279-289.	2.8	27
1465	Unraveling Stable Vanadium Tetraboride and Triboride by First-Principles Computations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21649-21657.	1.5	33
1466	Lithium migration at low concentration in TiO_2 polymorphs. <i>Computational and Theoretical Chemistry</i> , 2015, 1072, 43-51.	1.1	19
1467	Structural Difference in Superconductive and Nonsuperconductive $Bi^{\pm}S$ Planes within $Bi_4O_4Bi_2S_4$ Blocks. <i>Inorganic Chemistry</i> , 2015, 54, 10462-10467.	1.9	10
1468	Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TM = Cr, Ni, Ta and Zr) alloys. <i>Materials Chemistry and Physics</i> , 2015, 162, 748-756.	2.0	17

#	ARTICLE	IF	CITATIONS
1469	Oriented PrBaCo ₂ O ₅ + δ thin films for solid oxide fuel cells. <i>Journal of Power Sources</i> , 2015, 278, 623-629.	4.0	26
1470	Facile synthesis of PbWO ₄ : Applications in photoluminescence and photocatalytic degradation of organic dyes under visible light. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 348-355.	2.0	36
1471	Adsorption and dissociation of ammonia on small iron clusters. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 346-352.	3.8	23
1472	Structure, Superconductivity, and Magnetism of Ce(O,F)BiS ₂ Single Crystals. <i>Crystal Growth and Design</i> , 2015, 15, 39-44.	1.4	32
1473	First-principles study of Rashba effect in the (LaAlO ₃) ₂ /(SrTiO ₃) ₂ . <i>Molecular Simulation</i> , 2015, 41, 923-926.	0.9	1
1474	Free volume structure of realgar β -As ₄ S ₄ by positron annihilation lifetime spectroscopy. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 79, 49-54.	1.9	17
1475	Comprehensive model of metadislocation movement in Al ₁₃ Co ₄ . <i>Scripta Materialia</i> , 2015, 98, 24-27.	2.6	12
1476	Mechanism of enhanced photocatalytic activities on N-doped La ₂ Ti ₂ O ₇ : An insight from density-functional calculations. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 980-989.	3.8	27
1477	Synthesis and crystal structure analysis of Li ₂ NaBP ₂ O ₈ and LiNa ₂ B ₅ P ₂ O ₁₄ . <i>Journal of Solid State Chemistry</i> , 2015, 225, 65-71.	1.4	18
1478	Insights into the interaction between CH ₂ F ₂ and titanium dioxide: DRIFT spectroscopy and DFT analysis of the adsorption energetics. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1614-1620.	2.0	6
1479	Spectroscopic investigations on SrAl ₂ O ₄ polymorphs. <i>Journal of Luminescence</i> , 2015, 159, 158-165.	1.5	8
1480	Photoluminescence properties of Eu ³⁺ -activated CaMoO ₄ phosphors for WLEDs applications and its Judd-Ofelt analysis. <i>Journal of Materials Science</i> , 2015, 50, 287-298.	1.7	70
1481	Electronic and magnetic properties of Fe(Mn)-doped Cd and Zn nitrides for spintronic applications: a first-principles study. <i>Journal of Materials Science</i> , 2015, 50, 1446-1456.	1.7	8
1482	Scheelite-type MWO ₄ (M=Ca, Sr, and Ba) nanophosphors: Facile synthesis, structural characterization, photoluminescence, and photocatalytic properties. <i>Materials Research Bulletin</i> , 2015, 61, 422-432.	2.7	66
1483	On stoichiometry and intermixing at the spinel/perovskite interface in CoFe ₂ O ₄ /BaTiO ₃ thin films. <i>Nanoscale</i> , 2015, 7, 218-224.	2.8	17
1484	Novel nanosynthesis of In ₂ O ₃ and its application as a resistive gas sensor for sevoflurane anesthetic. <i>Journal of Materials Chemistry B</i> , 2015, 3, 399-407.	2.9	21
1485	Crystal structure analysis of Na ₄ Si ₄ Ge by single crystal X-ray diffraction. <i>Journal of Alloys and Compounds</i> , 2015, 623, 473-479.	2.8	11
1486	CaTiO ₃ :Eu ³⁺ , a potential red long lasting phosphor: Energy migration and characterization of trap level distribution. <i>Journal of Alloys and Compounds</i> , 2015, 622, 1068-1073.	2.8	41

#	ARTICLE	IF	CITATIONS
1487	Synthesis and crystal structure investigations of ternary oxides in the Na-Pu-O system. Journal of Nuclear Materials, 2015, 457, 54-62.	1.3	16
1488	Silicene on Ag(111): Geometric and electronic structures of a new honeycomb material of Si. Progress in Surface Science, 2015, 90, 1-20.	3.8	58
1489	Energetics of non-covalent interactions from electron and energy density distributions. Computational and Theoretical Chemistry, 2015, 1053, 53-59.	1.1	64
1490	The Sr-poor part of the Sr-Pd,Pt-Si,Ge systems: Phase equilibria and crystal structure of ternary phases. Journal of Alloys and Compounds, 2015, 618, 656-665.	2.8	3
1491	Anomalous phonon stiffening associated with the (1 1 1) antiphase boundary in L12 Ni3Al. Acta Materialia, 2015, 82, 287-294.	3.8	29
1492	Sr3Bi2(SeO3)6·H2O: A novel anionic layer consisting of second-order Jahn-Teller (SOJT) distortive cations. Journal of Solid State Chemistry, 2015, 221, 73-78.	1.4	8
1493	Structural trends in hybrid perovskites [Me2NH2]M(HCOO)3 (M = Ti, Sn, Pb). Journal of Materials Chemistry, 2015, 25, 295-298.	1.3	29
1494	Preparation and investigation of CaZr4(PO4)6:Dy3+ single-phase full-color phosphor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 1-6.	2.0	50
1495	A Review of X-Ray Absorption Near-Edge Spectroscopic Studies of Pyrochlore-Type Oxides Proposed for Nuclear Materials Applications. , 2016, , .		1
1496	Flexible Yttrium Coordination Geometry Inhibits Bare-Metal-Guest Interactions in the Metal-Organic Framework Y(btc). Energies, 2016, 9, 836.	1.6	0
1497	Oxygen Evolution at Manganite Perovskite Ruddlesden-Popper Type Particles: Trends of Activity on Structure, Valence and Covalence. Materials, 2016, 9, 921.	1.3	34
1498	Origin of the unidentified positive mobile ions causing the bias temperature instability in SiC MOSFETs and their diffusion process. Applied Physics Express, 2016, 9, 064301.	1.1	7
1499	Structural transitions and electronic properties of sodium superoxide at high pressures. RSC Advances, 2016, 6, 67910-67915.	1.7	5
1500	Disclosing the electronic structure and optical properties of Ag4V2O7 crystals: experimental and theoretical insights. CrystEngComm, 2016, 18, 6483-6491.	1.3	15
1501	Nitrogen-Rich Manganese Oxynitrides with Enhanced Catalytic Activity in the Oxygen Reduction Reaction. Angewandte Chemie, 2016, 128, 8095-8099.	1.6	8
1502	Superconductivity phase diagram of Se-substituted CeO0.5F0.5Bi(S1-xSex)2. Journal of Physics: Conference Series, 2016, 683, 012001.	0.3	9
1503	Ax(H3O)2·xMn5(HPO3)6 (A = Li, Na, K and NH4): open-framework manganese(ii) phosphites templated by mixed cationic species. Dalton Transactions, 2016, 45, 12188-12199.	1.6	3
1504	Recent Advances in Layered Metal Chalcogenides as Superconductors and Thermoelectric Materials: Fe-Based and Bi-Based Chalcogenides. Chemical Record, 2016, 16, 633-651.	2.9	15

#	ARTICLE	IF	CITATIONS
1505	Quaternary Iodide $K(\text{Ca,Sr})\text{I}_3:\text{Eu}^{2+}$ Single-Crystal Scintillators for Radiation Detection: Crystal Structure, Electronic Structure, and Optical and Scintillation Properties. <i>Advanced Optical Materials</i> , 2016, 4, 1518-1532.	3.6	35
1506	First principles study of band line up at defective metal-oxide interface: oxygen point defects at Al/SiO_2 interface. <i>Journal Physics D: Applied Physics</i> , 2016, 49, 095304.	1.3	15
1507	Rapid and Energy-Saving Microwave-Assisted Solid-State Synthesis of Pr^{3+} , Eu^{3+} , or Tb^{3+} -Doped Lu_2O_3 Persistent Luminescence Materials. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 19593-19604.	4.0	75
1508	$\text{É}\text{TiO}$, a Novel Stable Polymorph of Titanium Monoxide. <i>Angewandte Chemie</i> , 2016, 128, 1684-1689.	1.6	3
1509	Charge distribution around BaO and TiO bonds in $\text{BaTi}_{1-x}\text{Zr}_x\text{O}_3$ through powder X-ray diffraction. <i>Rare Metals</i> , 2016, 40, 1.	3.6	3
1510	Thermoelectric properties of pnictogen-substituted skutterudites with alkaline-earth fillers using first-principles calculations. <i>Journal of Applied Physics</i> , 2016, 119, 205102.	1.1	8
1511	Oxidized Monolayers of Epitaxial Silicene on $\text{Ag}(111)$. <i>Scientific Reports</i> , 2016, 6, 22510.	1.6	9
1512	Magnetic structures and excitations in a multiferroic Y-type hexaferrite $\text{BaSrCo}_2\text{Fe}_{10}\text{O}_{22}$. <i>Physical Review B</i> , 2016, 94, .		
1513	Hexacoordinated nitrogen(V) stabilized by high pressure. <i>Scientific Reports</i> , 2016, 6, 36049.	1.6	10
1514	Inherent instability by antibonding coupling in AgSbTe_2 . <i>Japanese Journal of Applied Physics</i> , 2016, 55, 041801.	0.8	15
1515	Graphene based biosensors. <i>AIP Conference Proceedings</i> , 2016, , .	0.3	2
1516	Monolithic translucent $\text{BaMgAl}_{10}\text{O}_{17}:\text{Eu}^{2+}$ phosphors for laser-driven solid state lighting. <i>AIP Advances</i> , 2016, 6, .	0.6	28
1517	Crystalline-Amorphous-Crystalline Transformation in a Highly Brilliant Luminescent System with Trigonal-Planar Gold(I) Centers. <i>Scientific Reports</i> , 2016, 6, 26002.	1.6	16
1518	Play the heavy: An effective mass study for Fe_2O_3 and corundum oxides. <i>Journal of Chemical Physics</i> , 2016, 144, 164704.	1.2	28
1519	Room-temperature dynamic correlation between methylammonium molecules in lead-iodine based perovskites: An <i>ab initio</i> molecular dynamics perspective. <i>Physical Review B</i> , 2016, 94, .	1.1	62
1520	Theoretical and experimental investigation of defect formation / migration in $\text{Gd}_2\text{Ti}_2\text{O}_7$: General rule of oxide-ion migration in $\text{A}_2\text{B}_2\text{O}_7$ pyrochlore. <i>AIP Advances</i> , 2016, 6, .	0.6	21
1521	Thermomechanical response of thermoelectrics. <i>Applied Physics Letters</i> , 2016, 109, 223903.	1.5	23
1522	Determination of the basic physical properties of semiconductor chalcopyrite type MgSnT_2 ($T = \text{P, As, Sb}$) from first-principles calculations. <i>Journal of Materials Research</i> , 2016, 31, 1518-1531.	1.2	8

#	ARTICLE	IF	CITATIONS
1523	Polarization twist in perovskite ferrielectrics. <i>Scientific Reports</i> , 2016, 6, 32216.	1.6	26
1524	Atomic scale imaging of competing polar states in a Ruddlesden-Popper layered oxide. <i>Nature Communications</i> , 2016, 7, 12572.	5.8	26
1525	Enhancement of thermoelectric properties in the Nb-Co-Sn half-Heusler/Heusler system through spontaneous inclusion of a coherent second phase. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	29
1526	The effect of absorbed hydrogen on the dissolution of steel. <i>Heliyon</i> , 2016, 2, e00209.	1.4	33
1527	A review of defects and disorder in multinary tetrahedrally bonded semiconductors. <i>Semiconductor Science and Technology</i> , 2016, 31, 123004.	1.0	74
1528	Interstitial oxygen as a source of p-type conductivity in hexagonal manganites. <i>Nature Communications</i> , 2016, 7, 13745.	5.8	61
1529	Magnetism and magnetocrystalline anisotropy in single-layer PtSe ₂ : Interplay between strain and vacancy. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	51
1530	First-principles study of twin grain boundaries in epitaxial BaSi ₂ on Si(111). <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	22
1531	Synthesis, crystal structure, and properties of a perovskite-related bismuth phase, (NH ₄) ₃ Bi ₂ I ₉ . <i>APL Materials</i> , 2016, 4, .	2.2	106
1532	Compositional and temperature evolution of crystal structure of new thermoelectric compound La _{0.5} Bi ₂ S ₂ xSe _x . <i>Journal of Applied Physics</i> , 2016, 119, 155103.	1.1	29
1533	Bulk Superconductivity Induced by In-Plane Chemical Pressure Effect in Eu _{0.5} La _{0.5} FBiS ₂ xSe _x . <i>Journal of the Physical Society of Japan</i> , 2016, 85, 124708.	0.7	27
1534	A co-crystal between benzene and ethane: a potential evaporite material for Saturn's moon Titan. <i>IUCr</i> , 2016, 3, 192-199.	1.0	26
1535	Ba_2NiO_6 : A Dirac-Mott insulator with ferromagnetism near 100 K. <i>Physical Review B</i> , 2016, 94, .		55
1536	Persistence of polar distortion with electron doping in lone-pair driven ferroelectrics. <i>Physical Review B</i> , 2016, 94, .	1.1	50
1537	Biological applications of graphene oxide. <i>AIP Conference Proceedings</i> , 2016, , .	0.3	1
1538	High-throughput exploration of thermoelectric and mechanical properties of amorphous NbO ₂ with transition metal additions. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	11
1539	Crystallographic features related to a van der Waals coupling in the layered chalcogenide FePS ₃ . <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	41
1540	Counterion-Induced Variations in the Dimensionality and Topology of Uranyl Pimelate Complexes. <i>Crystal Growth and Design</i> , 2016, 16, 2826-2835.	1.4	40

#	ARTICLE	IF	CITATIONS
1541	Revealing the Reconstructed Surface of Li[Mn ₂]O ₄ . Nano Letters, 2016, 16, 2899-2906.	4.5	71
1542	Resolving the Physical Origin of Octahedral Tilting in Halide Perovskites. Chemistry of Materials, 2016, 28, 4259-4266.	3.2	211
1543	Microscopic interactions governing phase matchability in nonlinear optical materials. Journal of Materials Chemistry C, 2016, 4, 5858-5863.	2.7	6
1544	High Thermopower with Metallic Conductivity in <i>p</i> -Type Li-Substituted PbPdO ₂ . Chemistry of Materials, 2016, 28, 3367-3373.	3.2	25
1545	Preparation and Charge Density in (Co, Fe)-Doped La-Ca-Based Chromite. Journal of Electronic Materials, 2016, 45, 4364-4374.	1.0	2
1546	Novel High-Throughput Screening Approach for Functional Metal/Oxide Interfaces. Journal of Chemical Theory and Computation, 2016, 12, 1572-1582.	2.3	15
1547	Counter-ion control of structure in uranyl ion complexes with 2,5-thiophenedicarboxylate. CrystEngComm, 2016, 18, 1550-1562.	1.3	34
1548	A basin-hopping Monte Carlo investigation of the structural and energetic properties of 55- and 561-atom bimetallic nanoclusters: the examples of the ZrCu, ZrAl, and CuAl systems. Journal of Physics Condensed Matter, 2016, 28, 175302.	0.7	13
1549	Exploring the potential of Raman spectroscopy for crystallochemical analyses of complex hydrous silicates: II. Tourmalines. American Mineralogist, 2016, 101, 970-985.	0.9	61
1550	Effect of charge on point defect size misfits from ab initio: Aliovalently doped SrTiO_3 . Computational Materials Science, 2016, 119, 41-45.	1.4	5
1551	Theoretical and experimental study of octahedral tilting of Ca _{1-x} Gd _x MnO ₃ (x=0.05, 0.1, 0.15, 0.2) nanometric powders. Journal of Alloys and Compounds, 2016, 678, 219-227.	2.8	6
1552	Anchoring flexible uranyl dicarboxylate chains through stacking interactions of ancillary ligands on chiral U(<i>vi</i>) centres. CrystEngComm, 2016, 18, 3905-3918.	1.3	36
1553	Precipitation evolution and hardening in Mg Sm Zn Zr alloys. Acta Materialia, 2016, 111, 335-347.	3.8	102
1554	Electronic structure and lattice dynamics of rhombohedral BiAlO ₃ from first-principles. Materials Chemistry and Physics, 2016, 177, 405-412.	2.0	16
1555	Capturing Phase Evolution during Solvothermal Synthesis of Metastable Cu ₄ O ₃ . Chemistry of Materials, 2016, 28, 3080-3089.	3.2	22
1556	Peculiarities of thermoelectric half-Heusler phase formation in Gd-Ni-Sb and Lu-Ni-Sb ternary systems. Journal of Solid State Chemistry, 2016, 239, 145-152.	1.4	25
1557	Safe P ₄ reagent in a reusable porous coordination network. Dalton Transactions, 2016, 45, 6357-6360.	1.6	25
1558	Thermoelectric properties of new Bi-chalcogenide layered compounds. Cogent Physics, 2016, 3, .	0.7	31

#	ARTICLE	IF	CITATIONS
1559	Pseudocapacitance and excellent cyclability of 2,5-dimethoxy-1,4-benzoquinone on graphene. <i>Energy and Environmental Science</i> , 2016, 9, 2586-2594.	15.6	129
1560	Valence charge density of multi-doped Mg ₂ Si thermoelectric materials from maximum entropy method analysis. <i>Journal of Alloys and Compounds</i> , 2016, 681, 66-74.	2.8	2
1561	Anti-site mixing governs the electrochemical performances of olivine-type MgMnSiO ₄ cathodes for rechargeable magnesium batteries. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13524-13529.	1.3	39
1562	High dielectric constant and capacitance in ultrasmall (2.5 nm) SrHfO ₃ perovskite nanoparticles produced in a low temperature non-aqueous sol-gel route. <i>RSC Advances</i> , 2016, 6, 51493-51502.	1.7	19
1563	Achirality in the low temperature structure and lattice modes of tris(acetylacetonate)iron(III). <i>Dalton Transactions</i> , 2016, 45, 8278-8283.	1.6	0
1564	Understanding and Tuning the Hydrogen Evolution Reaction on Pt-Covered Tungsten Carbide Cathodes. <i>Journal of the Electrochemical Society</i> , 2016, 163, F629-F636.	1.3	15
1565	Field-insensitive heavy fermion features and phase transition in the caged-structure quasi-skutterudite Sm ₃ Ru ₄ Ge ₁₃ . <i>Journal of Alloys and Compounds</i> , 2016, 669, 254-261.	2.8	5
1566	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb ₂ O ₆ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 9604-9611.	1.5	25
1567	Coincidence Lattices of 2D Crystals: Heterostructure Predictions and Applications. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10895-10908.	1.5	68
1568	Metallic back-contact interface design in photoelectrochemical devices. <i>Journal of Materials Chemistry C</i> , 2016, 4, 8989-8996.	2.7	7
1569	Analogies between Jahn-Teller and Rashba spin physics. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1442-1450.	1.0	3
1570	Compressional behavior of omphacite to 47 GPa. <i>Physics and Chemistry of Minerals</i> , 2016, 43, 707-715.	0.3	9
1571	Improving the photocatalytic activity of s-triazine based graphitic carbon nitride through metal decoration: an ab initio investigation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26466-26474.	1.3	16
1572	Crystal, electronic, and magnetic structures of M ₂ AgF ₄ (M = Na-Cs) phases as viewed from the DFT+U method. <i>Dalton Transactions</i> , 2016, 45, 16255-16261.	1.6	13
1573	Domains and ferroelectric switching pathways in Ca ₃ O ₇ from first principles. <i>Physical Review B</i> , 2016, 94, .	1.1	58
1574	Characterizing magnesium-silicon binaries in Al-Mg-Si supersaturated solid solution by first-principles calculations. <i>Journal of Science: Advanced Materials and Devices</i> , 2016, 1, 527-530.	1.5	3
1575	Layered amorphous silicon as negative electrodes in lithium-ion batteries. <i>Journal of Power Sources</i> , 2016, 332, 290-298.	4.0	30
1576	Structural stability and magnetic properties of WFeH phases. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 13093-13100.	3.8	15

#	ARTICLE	IF	CITATIONS
1577	Manipulating electrochemical performance through doping beyond the solubility limit. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16098-16105.	1.3	13
1579	Extended Intermolecular Interactions Governing Photocurrentâ€œVoltage Relations in Ternary Organic Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3936-3944.	2.1	11
1580	Electronic Structure of Catalysis Intermediates by the GOW0 Approximation. <i>Catalysis Letters</i> , 2016, 146, 2009-2014.	1.4	15
1581	First-principles calculations on structure and properties of amorphous Li ₅ P ₄ O ₈ N ₃ (LiPON). <i>Journal of Power Sources</i> , 2016, 331, 382-390.	4.0	33
1582	A Structural Investigation of Hydrus and Anhydrous Rare-Earth Phosphates. <i>Inorganic Chemistry</i> , 2016, 55, 9685-9695.	1.9	37
1584	Yb ₉ CuMg ₄ (x = 0.034): A β -Phase Formed by Lanthanoids. <i>Inorganic Chemistry</i> , 2016, 55, 8174-8183.	1.9	7
1585	Static magnetic order on the metallic triangular lattice in CrSe ₂ . <i>Physical Review B</i> , 2016, 94, 114411.	1.1	13
1586	First-principles analysis on role of spinel (111) phase boundaries in Li _{4+3x} Ti ₅ O ₁₂ Li-ion battery anodes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23383-23388.	1.3	17
1587	Structure, properties, and disorder in the new distorted-Hollandite Pb ₄ Se ₈ . <i>Journal of Solid State Chemistry</i> , 2016, 242, 112-119.	1.4	7
1588	The effect of partial substitution of Ni by Mg on the structural, magnetic and spectroscopic properties of the double perovskite Sr ₂ NiTeO ₆ . <i>Dalton Transactions</i> , 2016, 45, 14378-14393.	1.6	19
1589	Crystal and electronic structure changes during the charge-discharge process of Na ₄ Co ₃ (PO ₄) ₂ P ₂ O ₇ . <i>Journal of Power Sources</i> , 2016, 326, 220-225.	4.0	32
1590	A thin film of a type II Ge clathrate epitaxially grown on a Ge substrate. <i>CrystEngComm</i> , 2016, 18, 5630-5638.	1.3	18
1591	Design of nanoconfined MWNTs@NaTi ₂ (PO ₄) ₃ coaxial cables with superior rate capability and long-cycle life for Na-ion batteries. <i>Applied Materials Today</i> , 2016, 4, 54-61.	2.3	24
1592	Estimation of spectroscopic parameters and colour purity of the red-light-emitting YBa ₃ B ₉ O ₁₈ phosphor: Juddâ€œOfelt approach. <i>Journal of Luminescence</i> , 2016, 180, 169-176.	1.5	21
1593	Conversion of Single Crystalline Pb ₂ to CH ₃ NH ₃ Pb ₃ : Structural Relations and Transformation Dynamics. <i>Chemistry of Materials</i> , 2016, 28, 6501-6510.	3.2	76
1594	The role of nonmagnetic d ₀ vs. d ₁₀ B-type cations on the magnetic exchange interactions in osmium double perovskites. <i>Journal of Solid State Chemistry</i> , 2016, 243, 119-123.	1.4	19
1595	Tuning the Phase Stability of Sodium Metal Pyrophosphates for Synthesis of High Voltage Cathode Materials. <i>Chemistry of Materials</i> , 2016, 28, 6724-6730.	3.2	14
1596	Ga-Promoted Photocatalytic H ₂ Production over Pt/ZnO Nanostructures. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 23729-23738.	4.0	43

#	ARTICLE	IF	CITATIONS
1597	Determination of the local structure of CsBi ₄ Pb _x Te ₆ (x = 0, 1, 2, 3, 4) by EXAFS and Rietveld refinement. <i>Journal of Materials Chemistry A</i> , 2016, 4, 14371-14379.	1.3	4
1598	Chemical Pressure-Driven Incommensurability in CaPd ₅ : Clues to High-Pressure Chemistry Offered by Complex Intermetallics. <i>Inorganic Chemistry</i> , 2016, 55, 6781-6793.	1.9	17
1599	Experimental and first-principles DFT study on the electrochemical reactivity of garnet-type solid electrolytes with carbon. <i>Journal of Materials Chemistry A</i> , 2016, 4, 14371-14379.	5.2	25
1600	Effects of strain on the stability of tetragonal ZrO ₂ . <i>Physical Review B</i> , 2016, 94, .	1.8	18
1601	Understanding sodium-ion diffusion in layered P2 and P3 oxides via experiments and first-principles calculations: a bridge between crystal structure and electrochemical performance. <i>NPG Asia Materials</i> , 2016, 8, e266-e266.	3.8	101
1602	Chromate adsorption mechanism on nanodiamond-derived onion-like carbon. <i>Journal of Hazardous Materials</i> , 2016, 320, 368-375.	6.5	25
1603	Co-adsorption of O ₂ and H ₂ O on Al(111) surface: a vdW-DFT study. <i>RSC Advances</i> , 2016, 6, 79836-79843.	1.7	14
1604	Soft chemical synthesis and crystal structure of novel hydrogen titanium oxide H ₂ Ti ₁₂ O ₂₅ . <i>Journal of the Ceramic Society of Japan</i> , 2016, 124, 710-713.	0.5	9
1605	Oriented growth and electrical property of LiAl ₅ O ₈ film by laser chemical vapor deposition. <i>Journal of the Ceramic Society of Japan</i> , 2016, 124, 111-115.	0.5	5
1606	Analytical ABF-STEM imaging of Li ions in rechargeable batteries. <i>Microscopy (Oxford, England)</i> , 2016, 66, 25-38.	0.7	11
1607	Direct Observation of Reversible Transformation of CH ₃ NH ₃ Pb ₃ and NH ₄ Pb ₃ Induced by Polar Gaseous Molecules. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5068-5073.	2.1	62
1608	Synthesis, crystal structure and temperature dependent luminescence of Eu ³⁺ doped SrGd ₂ O ₄ host: An approach towards tunable red emissions for display applications. <i>Ceramics International</i> , 2016, 42, 18536-18546.	2.3	23
1609	Structural, magnetic and optical characterization of Ni _{0.8} Zn _{0.2} Fe ₂ O ₄ nano particles prepared by co-precipitation method. <i>Physica B: Condensed Matter</i> , 2016, 502, 181-186.	1.3	13
1610	Weak Ferromagnetism and Multiple Metamagnetic Transitions in the Non-centrosymmetric Tetragonal Compound CePdSi ₃ . <i>Journal of the Physical Society of Japan</i> , 2016, 85, 104703.	0.7	9
1611	Phonon transport in the ground state of two-dimensional silicon and germanium. <i>RSC Advances</i> , 2016, 6, 69956-69965.	1.7	20
1612	First-principles study of the cubic CaHfO ₃ (001) surface. <i>International Journal of Modern Physics B</i> , 2016, 30, 1650168.	1.0	5
1613	First-principles study of interface magnetic structure in Nd ₂ Fe ₁₄ B/(Fe,Co) exchange spring magnets. <i>Physical Review B</i> , 2016, 93, .	1.1	12
1614	Magnetoelectric effect and magnetic phase diagram of a polar ferrimagnet CaBaFe ₄ O ₇ . <i>Physical Review B</i> , 2016, 93, .	1.1	19

#	ARTICLE	IF	CITATIONS
1615	Temperature-dependent high energy-resolution EELS of ferroelectric and paraelectric BaTiO_3 . Physical Review B, 2016, 93, .	1.1	14
1616	Electromagnon excitation in the field-induced noncollinear ferrimagnetic phase of Ba_2O studied by polarized inelastic neutron scattering and terahertz time-domain optical spec. Physical Review B, 2016, 93, .	1.1	14
1617	Observation of magnetic order in multiferroic SmMn_2O_5 studied by resonant x-ray magnetic scattering. Physical Review B, 2016, 93, .	1.1	17
1618	Low-temperature crystal and magnetic structure of $\text{Sr}_2\text{Mn}_2\text{O}_7$. Physical Review B, 2016, 93, .	1.1	14
1619	Unconventional magnetism on a honeycomb lattice in $\text{Sr}_2\text{Mn}_2\text{O}_7$ by muon spin rotation. Physical Review B, 2016, 94, .	1.1	14
1620	Synthesis and characterization of some ferrite nanoparticles prepared by co-precipitation method. Journal of Materials Science: Materials in Electronics, 2016, 27, 12000-12008.	1.1	26
1621	<i>Ab initio</i> study of the ferroelectric strain dependence and walls in the barium metal fluorides BaMgF_4 and BaZnF_4 . Physical Review B, 2016, 93, .	1.1	9
1622	Magnetic ordering in pressure-induced phases with giant spin-driven ferroelectricity in multiferroic TbMnO_3 . Physical Review B, 2016, 93, .	1.1	22
1623	Structure and Curie temperature relationships in ferroelectric perovskites: Anomalous behavior of BaTiO_3 . Physical Review B, 2016, 93, .	1.1	39
1624	DFT, statistical inference, and experiments: Pressure dependence of the structure and electronic properties of $\text{Sr}_2\text{Mn}_2\text{O}_7$. Physical Review B, 2016, 93, .	1.1	21
1625	Magnetic properties of $\text{Fe}_{1-x}\text{P}_x\text{S}_x\text{Co}$ and its alloys with P, S, and Co. Physical Review B, 2016, 93, .	1.1	27
1626	Electronic structure of interstitial hydrogen in lutetium oxide from DFT and comparison study with UO_2 . Physical Review B, 2016, 94, .	1.1	21
1627	Quantum Tunneling of Water in Beryl: A New State of the Water Molecule. Physical Review Letters, 2016, 116, 167802.	2.9	92
1628	Tetrahydrofuran tetracarboxylic Acid: An Isomerizable Framework-Forming Ligand in Homo- and Heterometallic Complexes with UO_2^{2+} , Ag^+ , and Pb^{2+} . Crystal Growth and Design, 2016, 16, 7083-7093.	1.4	22
1629	First-principles study of structural and surface properties of (001) and (010) surfaces of hydroxylapatite and carbonated hydroxylapatite. Journal of Applied Crystallography, 2016, 49, 1893-1903.	1.9	22
1630	Coexistence of Superconductivity and Superhardness in Beryllium Hexaboride Driven by Inherent Multicenter Bonding. Journal of Physical Chemistry Letters, 2016, 7, 4898-4904.	2.1	16
1631	Regulation of NO Uptake in Flexible Ru Dimer Chain Compounds with Highly Electron Donating Dopants. Inorganic Chemistry, 2016, 55, 12085-12092.	1.9	10
1632	Design and synthesis of the superionic conductor $\text{Na}_{10}\text{Sn}_2\text{P}_{12}\text{S}_{12}$. Nature Communications, 2016, 7, 11009.	5.8	246

#	ARTICLE	IF	CITATIONS
1633	Microstructural Analysis of Perfluoropentacene Films on Graphene and Graphite: Interface-Mediated Alignment and Island Formation. <i>Crystal Growth and Design</i> , 2016, 16, 6941-6950.	1.4	6
1634	Density functional theory based tight binding study on theoretical prediction of low-density nanoporous phases ZnO semiconductor materials. <i>Journal of Physics: Conference Series</i> , 2016, 726, 012022.	0.3	7
1635	The separation mechanism of Am(^{III}) from Eu(^{III}) by diglycolamide and nitrilotriacetamide extraction reagents using DFT calculations. <i>Dalton Transactions</i> , 2016, 45, 17530-17537.	1.6	35
1636	Chemical bonding and charge density distribution analysis of undoped and lanthanum doped barium titanate ceramics. <i>Journal of Chemical Sciences</i> , 2016, 128, 1913-1921.	0.7	13
1637	Theoretical Insights into the Effects of Oxidation and Mo-Doping on the Structure and Stability of Pt-Ni Nanoparticles. <i>Nano Letters</i> , 2016, 16, 7748-7754.	4.5	64
1638	Structural evaluations and temperature dependent photoluminescence characterizations of Eu ³⁺ -activated SrZrO ₃ hollow spheres for luminescence thermometry applications. <i>Scientific Reports</i> , 2016, 6, 25787.	1.6	44
1639	Cation Distribution Analysis of Ca-La-Co M-type Ferrites by Neutron Diffraction, Extended X-ray Absorption Fine Structure and X-ray Magnetic Circular Dichroism. <i>Funtai Oyobi Fumatsu Yakin/Journal of the Japan Society of Powder and Powder Metallurgy</i> , 2016, 63, 101-108.	0.1	8
1640	Syntheses of Novel Metal Hydrides under High Pressure and High Temperature. <i>Funtai Oyobi Fumatsu Yakin/Journal of the Japan Society of Powder and Powder Metallurgy</i> , 2016, 63, 298-305.	0.1	2
1641	Development of Opposed-Type Anvils with Wide-Angle Aperture and Investigation of Pressure-Induced Phase Transition of Ca(OD) ₂ . <i>Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu</i> , 2016, 26, 128-139.	0.1	0
1642	Phase-Transition Studies on Earth's Materials by High-Pressure Experiments and Calorimetry, and Crystal-Chemical Studies on High-Pressure Inorganic Compounds. <i>Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu</i> , 2016, 26, 167-177.	0.1	0
1643	Efficient automatic screening for Li ion conductive inorganic oxides with bond valence pathway models and percolation algorithm. <i>Japanese Journal of Applied Physics</i> , 2016, 55, 01AH05.	0.8	17
1644	Emergence of Negative Capacitance in Multidomain Ferroelectric/Paraelectric Nanocapacitors at Finite Bias. <i>Advanced Materials</i> , 2016, 28, 335-340.	11.1	30
1645	Ohmic Contacts to 2D Semiconductors through van der Waals Bonding. <i>Advanced Electronic Materials</i> , 2016, 2, 1500405.	2.6	91
1646	ZrB ₂ -ZrC _x N _{1-x} Eutectic Composites Produced by Melt Solidification. <i>Journal of the American Ceramic Society</i> , 2016, 99, 667-673.	1.9	9
1647	Mechanical alloying-spark plasma sintering synthesis and thermoelectric properties of n-type NiSe _{2+x} semiconductors: analysis of intrinsic defects and phase structures. <i>Journal of Materials Science: Materials in Electronics</i> , 2016, 27, 8363-8369.	1.1	4
1648	Structural characterization and electron density distribution studies of (La _{0.8} Ca _{0.2})(Cr _{0.9-x} Co _{0.1Mnx})O ₃ . <i>Physica B: Condensed Matter</i> , 2016, 493, 25-34.	1.3	4
1649	High-Pressure Polymorph of NaBiO ₃ . <i>Inorganic Chemistry</i> , 2016, 55, 5747-5749.	1.9	7
1650	Energy Landscape of Molecular Motion in Cubic Methylammonium Lead Iodide from First-Principles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12403-12410.	1.5	57

#	ARTICLE	IF	CITATIONS
1651	High-pressure behavior of the polymorphs of FeOOH. <i>American Mineralogist</i> , 2016, 101, 1483-1488.	0.9	8
1652	Synthesis, crystal structures, and magnetic properties of double perovskites SrLaNiOsO ₆ and BaLaNiOsO ₆ . <i>Solid State Communications</i> , 2016, 243, 49-54.	0.9	15
1653	Modulation of the Structure and Properties of Uranyl Ion Coordination Polymers Derived from 1,3,5-Benzenetriacetate by Incorporation of Ag(I) or Pb(II). <i>Inorganic Chemistry</i> , 2016, 55, 6799-6816.	1.9	42
1654	Band Gaps of the Lead-Free Halide Double Perovskites Cs ₂ BiAgCl ₆ and Cs ₂ BiAgBr ₆ from Theory and Experiment. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2579-2585.	2.1	529
1655	Order of the transition metal layer in LiNi _{1/3} Co _{1/3} Mn _{1/3} O ₂ and stability of the crystal structure. <i>Ionics</i> , 2016, 22, 991-995.	1.2	9
1656	Facet control of ceria nanocrystals synthesized by an oleate-modified hydrothermal method. <i>Advanced Powder Technology</i> , 2016, 27, 64-71.	2.0	6
1657	Theoretical study of structural characteristics, mechanical properties and electronic structure of metal (TM = V, Nb and Ta) silicides. <i>Journal of Alloys and Compounds</i> , 2016, 681, 412-420.	2.8	33
1658	Magnetic ordering and crystal field effects in quasi-caged structure compound PrFe ₂ Al ₈ . <i>Journal of Physics and Chemistry of Solids</i> , 2016, 91, 69-75.	1.9	11
1659	Magnetic interactions in new fluorite-related rare earth oxides LnLn TM 2RuO ₇ (Ln, Ln TM =rare earths). <i>Journal of Solid State Chemistry</i> , 2016, 239, 214-219.	1.4	7
1660	Preparation of rutile TiO ₂ by hydrolysis of TiOCl ₂ solution: experiment and theory. <i>RSC Advances</i> , 2016, 6, 59541-59549.	1.7	13
1661	A DFT study of the adsorption of O ₂ and H ₂ O on Al(111) surfaces. <i>RSC Advances</i> , 2016, 6, 56303-56312.	1.7	37
1662	Chiral and achiral copper(II) complexes: structure, bonding and biological activities. <i>RSC Advances</i> , 2016, 6, 59055-59065.	1.7	24
1663	High-Speed Preparation of Highly (100)-Oriented CeO ₂ Film by Laser Chemical Vapor Deposition. <i>Journal of the American Ceramic Society</i> , 2016, 99, 3104-3110.	1.9	3
1664	Quasi-Two-Dimensional Magnetism in Co-Based Shandites. <i>Journal of the Physical Society of Japan</i> , 2016, 85, 064706.	0.7	26
1665	É ₂ TiO, a Novel Stable Polymorph of Titanium Monoxide. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 1652-1657.	7.2	42
1666	Nitrogen-Rich Manganese Oxynitrides with Enhanced Catalytic Activity in the Oxygen Reduction Reaction. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7963-7967.	7.2	52
1667	A New <i>n</i> = 4 Layered Ruddlesden-Popper Phase K _{2.5} Bi _{2.5} Ti ₄ O ₁₃ Showing Stoichiometric Hydration. <i>Inorganic Chemistry</i> , 2016, 55, 1403-1411.	1.9	14
1668	Probing structural adaptability in templated vanadium selenites. <i>Polyhedron</i> , 2016, 114, 184-193.	1.0	8

#	ARTICLE	IF	CITATIONS
1669	Layering effects on low frequency modes in n-layered MX ₂ transition metal dichalcogenides. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4807-4813.	1.3	18
1670	Synthesis, Crystal Structure, and Thermoelectric Properties of Na _{2+x} Al _{2+x} Sn ₄ ($x = 0.38, \epsilon = 0.24$). <i>Chemistry of Materials</i> , 2016, 28, 601-607.	3.2	7
1671	First-Principles Investigation of the Na ⁺ Ion Transport Property in Oxyfluorinated Titanium(IV) Phosphate Na ₃ Ti ₂ P ₂ O ₁₀ F. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1438-1445.	1.5	7
1672	Probing the electrochemical capacitance of MXene nanosheets for high-performance pseudocapacitors. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4460-4467.	1.3	65
1673	XRD and XAFS study on structure and cation valence state of layered ruthenium oxide electrodes, Li ₂ RuO ₃ and Li ₂ Mn _{0.4} Ru _{0.6} O ₃ , upon electrochemical cycling. <i>Solid State Ionics</i> , 2016, 285, 66-74.	1.3	30
1674	Computational Screening of Homovalent Lead Substitution in Organic-Inorganic Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2016, 120, 166-173.	1.5	208
1675	Synthesis and electrochemical properties of Li _{1.3} Nb _{0.3} V _{0.4} O ₂ as a positive electrode material for rechargeable lithium batteries. <i>Chemical Communications</i> , 2016, 52, 2051-2054.	2.2	76
1676	Interfacial electronic structure and charge transfer of hybrid graphene quantum dot and graphitic carbon nitride nanocomposites: insights into high efficiency for photocatalytic solar water splitting. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1050-1058.	1.3	57
1677	Segregation and Migration of the Oxygen Vacancies in the $\sqrt{3} \times \sqrt{3}$ (111) Tilt Grain Boundaries of Ceria. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6625-6632.	1.5	11
1678	Tungsten Bronze Barium Neodymium Titanate (Ba ₆ Nd _{8+2x} Ti ₁₈ O ₅₄): An Intrinsic Nanostructured Material and Its Defect Distribution. <i>Inorganic Chemistry</i> , 2016, 55, 3338-3350.	1.9	17
1679	Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1254-1259.	2.1	761
1680	Interstitial Oxide Ion Distribution and Transport Mechanism in Aluminum-Doped Neodymium Silicate Apatite Electrolytes. <i>Journal of the American Chemical Society</i> , 2016, 138, 4468-4483.	6.6	12
1681	The effect of hydrogen on the evolution of intergranular cracking: a cross-scale study using first-principles and cohesive finite element methods. <i>RSC Advances</i> , 2016, 6, 27282-27292.	1.7	19
1682	Real-space localization and quantification of hole distribution in chain-ladder Sr ₃ Ca ₁₁ Cu ₂₄ O ₄₁ superconductor. <i>Science Advances</i> , 2016, 2, e1501652.	4.7	20
1683	Sacrificial conversion of layered rare-earth hydroxide (LRH) nanosheets into (Y _{1-x} Eu _x)PO ₄ nanophosphors and investigation of photoluminescence. <i>Dalton Transactions</i> , 2016, 45, 5290-5299.	1.6	55
1684	Black Phosphorus as a High-Capacity, High-Capability Negative Electrode for Sodium-Ion Batteries: Investigation of the Electrode/Electrolyte Interface. <i>Chemistry of Materials</i> , 2016, 28, 1625-1635.	3.2	238
1685	Uranyl Ion Complexes with Long-Chain Aliphatic β -Dicarboxylates and 3d-Block Metal Counterions. <i>Inorganic Chemistry</i> , 2016, 55, 2133-2145.	1.9	30
1686	Surface Properties of CH ₃ NH ₃ Pb ₃ for Perovskite Solar Cells. <i>Accounts of Chemical Research</i> , 2016, 49, 554-561.	7.6	145

#	ARTICLE	IF	CITATIONS
1687	Investigation of the Na Intercalation Mechanism into Nanosized V_2O_5/C Composite Cathode Material for Na-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 6032-6039.	4.0	79
1688	Atomically resolved precipitates/matrix interfaces in $KTaO_3$ crystals. <i>Philosophical Magazine</i> , 2016, 96, 486-497.	0.7	3
1689	Synthesis and analysis of electron density distribution in $Ba_{1-x}Sr_xTiO_3$ ceramics. <i>Journal of Materials Science: Materials in Electronics</i> , 2016, 27, 2523-2533.	1.1	3
1690	Preparation of TaO_2 thin films using NbO_2 template layers by a pulsed laser deposition technique. <i>Thin Solid Films</i> , 2016, 599, 125-132.	0.8	7
1691	Surface functionalization of two-dimensional metal chalcogenides by Lewis acid-base chemistry. <i>Nature Nanotechnology</i> , 2016, 11, 465-471.	15.6	197
1692	XPS valence band studies of nanocrystalline Zr Pd alloy thin films. <i>Surface and Coatings Technology</i> , 2016, 303, 125-130.	2.2	14
1693	Effects of alloying elements and temperature on the elastic properties of W-based alloys by first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2016, 671, 267-275.	2.8	33
1694	Tailoring Magnetic Behavior in the Tb-Au-Si Quasicrystal Approximant System. <i>Inorganic Chemistry</i> , 2016, 55, 2001-2008.	1.9	23
1695	Silicene on Ag(111): Structure Evolution and Electronic Structure. <i>Springer Series in Materials Science</i> , 2016, , 143-165.	0.4	0
1696	Solution Combustion Synthesis, Characterization, and Photoelectrochemistry of $CuNb_2O_6$ and $ZnNb_2O_6$ Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16024-16034.	1.5	56
1697	$Li_3Mo_4P_5O_{24}$: A Two-Electron Cathode for Lithium-Ion Batteries with Three-Dimensional Diffusion Pathways. <i>Chemistry of Materials</i> , 2016, 28, 2229-2235.	3.2	20
1698	New-Structure-Type Fe-Based Superconductors: $Ca_xFe_4As_4$ ($x=0.784314$). <i>Chemical Society</i> , 2016, 138, 3410-3415.	6.6	228
1699	Ab initio study of pressure-induced phase transition, band gaps and X-ray photoemission valence band spectra of YVO_4 . <i>Computational Materials Science</i> , 2016, 117, 98-102.	1.4	2
1700	Structures and magnetic properties of new fluorite-related quaternary rare earth oxides LnY_2TaO_7 and $LaLn_2RuO_7$ (Ln =rare earths). <i>Journal of Solid State Chemistry</i> , 2016, 233, 37-43.	1.4	10
1701	Some new members of MAX family including light-elements: Nanolayered Hf_2XY ($X=Al, Si, P$ and $Y=B, C$). <i>Journal of Materials Chemistry</i> , 2016, 26, 1150-1155.	1.5	23
1702	Red-light-emitting inorganic La_2CaZnO_5 frameworks with high photoluminescence quantum efficiency: Theoretical approach. <i>Materials and Design</i> , 2016, 93, 203-215.	3.3	45
1703	Luminescence of undoped and Eu^{3+} doped nanocrystalline $SrWO_4$ scheelite: time resolved fluorescence complemented by DFT and positron annihilation spectroscopic studies. <i>RSC Advances</i> , 2016, 6, 3792-3805.	1.7	57
1704	Density functional theory study of $O-H$ and $C-H$ bond scission of methanol catalyzed by a chemisorbed oxygen layer on $Cu(111)$. <i>Surface Science</i> , 2016, 646, 288-297.	0.8	16

#	ARTICLE	IF	CITATIONS
1705	Investigation of the Thermal Stability of Nd _x Sc _y Zr _{1-x-y} O ₂ Materials Proposed for Inert Matrix Fuel Applications. <i>Inorganic Chemistry</i> , 2016, 55, 1032-1043.	1.9	7
1706	The effect of Mg ²⁺ incorporation on the structure of calcium carbonate clusters: investigation by the anharmonic downward distortion following method. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2690-2698.	1.3	20
1707	An ab initio study on electronic and magnetic properties of Cr, V doped Cd and Zn nitrides for spintronic applications. <i>Journal of Magnetism and Magnetic Materials</i> , 2016, 406, 48-59.	1.0	11
1708	An implementation of artificial neural-network potentials for atomistic materials simulations: Performance for TiO ₂ . <i>Computational Materials Science</i> , 2016, 114, 135-150.	1.4	377
1709	Tuning Phosphorene Nanoribbon Electronic Structure through Edge Oxidization. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2149-2158.	1.5	28
1710	Nanoscale cross-correlated AFM, Kelvin probe, elastic modulus and quantum mechanics investigation of clay mineral surfaces: The case of chlorite. <i>Applied Clay Science</i> , 2016, 131, 175-181.	2.6	30
1711	Association of defects in doped non-stoichiometric ceria from first principles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3804-3811.	1.3	35
1712	Hydrothermal Synthesis, Crystal Structure, and Superconductivity of a Double-Perovskite Bi Oxide. <i>Chemistry of Materials</i> , 2016, 28, 459-465.	3.2	54
1713	Local atomic arrangement and scintillation properties of Eu- and Ce-doped NaY ₂ O ₇ . <i>Journal of Solid State Chemistry</i> , 2016, 233, 103-107.	1.4	6
1714	Synthesis and characterization of metastable β -Ag ₂ WO ₄ : an experimental and theoretical approach. <i>Dalton Transactions</i> , 2016, 45, 1185-1191.	1.6	24
1715	Br ₂ induced oxidative pore modification of a porous coordination network. <i>Dalton Transactions</i> , 2016, 45, 489-493.	1.6	21
1716	Structures and optical absorption of Bi ₂ O ₃ and LaOBi ₂ O ₇ . <i>Solid State Communications</i> , 2016, 227, 19-22.	0.9	35
1717	Understanding the thermodynamic pathways of SnO-to-SnO _x phase transition. <i>Computational Materials Science</i> , 2016, 111, 359-365.	1.4	22
1718	The role of inorganic acidity on templated vanadate composition and dimensionality. <i>Journal of Solid State Chemistry</i> , 2016, 236, 215-221.	1.4	4
1719	Luminescence investigation of R ³⁺ -doped alkaline earth tungstates prepared by a soft chemistry method. <i>Journal of Luminescence</i> , 2016, 170, 736-742.	1.5	21
1720	Real-Time Molecular Visualization Supporting Diffuse Interreflections and Ambient Occlusion. <i>IEEE Transactions on Visualization and Computer Graphics</i> , 2016, 22, 718-727.	2.9	12
1721	Scintillation properties of Eu ²⁺ -doped KBa ₂ Bi ₅ and K ₂ Ba ₄ . <i>Journal of Luminescence</i> , 2016, 169, 301-307.	1.5	23
1722	Effect of nitrogen doping on titanium carbonitride-derived adsorbents used for arsenic removal. <i>Journal of Hazardous Materials</i> , 2016, 302, 375-385.	6.5	24

#	ARTICLE	IF	CITATIONS
1723	Structure and magnetic properties of flux grown single crystals of $\text{Co}_3\text{FeSn}_2\text{S}_2$ shandites. Journal of Solid State Chemistry, 2016, 233, 8-13.	1.4	31
1724	Short review of high-pressure crystal growth and magnetic and electrical properties of solid-state osmium oxides. Journal of Solid State Chemistry, 2016, 236, 45-54.	1.4	14
1725	Synthesis of new fluorite-related rare earth oxides Ln_2MO_7 (Ln, Tj) Ln_2MO_7 (Ln, Tj). Journal of Thermal Analysis and Calorimetry, 2017, 127, 749-754.	2.0	2
1726	Structural, elastic and magnetic properties of Mn and Sb doped chromium nitride – An ab initio study. Materials Chemistry and Physics, 2017, 192, 291-298.	2.0	10
1727	AgBi_4 as a Lead-Free Solar Absorber with Potential Application in Photovoltaics. Chemistry of Materials, 2017, 29, 1538-1549.	3.2	102
1728	Understanding Local Defects in Li-Ion Battery Electrodes through Combined DFT/NMR Studies: Application to LiVPO_4F . Journal of Physical Chemistry C, 2017, 121, 3219-3227.	1.5	37
1729	Preparation of Mo-Re-C samples containing Mo ₇ Re ₁₃ C with the $\hat{\Gamma}$ -Mn-type structure by solid state reaction of planetary-ball-milled powder mixtures of Mo, Re and C, and their crystal structures and superconductivity. Journal of Solid State Chemistry, 2017, 245, 207-212.	1.4	0
1730	Crystallographic, magnetic and electrical characteristics of $\text{R}_3\text{Ni}_8\text{Sn}_4$ compounds (R = Y, Nd, Sm, Gd). Journal of Solid State Chemistry, 2017, 245, 207-212.	2.8	2
1731	Coordination Polymers and Cage-Containing Frameworks in Uranyl Ion Complexes with <i>rac</i> - and (1 <i>R</i> ,2 <i>R</i>)- <i>trans</i> -1,2-Cyclohexanedicarboxylates: Consequences of Chirality. Inorganic Chemistry, 2017, 56, 1455-1469.	1.9	37
1732	Ab initio study of the structure and stability of $\text{CaMg}(\text{CO}_3)_2$ at high pressure. American Mineralogist, 2017, 102, 210-215.	0.9	13
1733	Structure analysis of vitusite glass – ceramic waste forms using extended X-ray absorption fine structures. Ceramics International, 2017, 43, 4687-4691.	2.3	5
1734	Ab initio insight into graphene nanofibers to destabilize hydrazine borane for hydrogen release. Chemical Physics Letters, 2017, 669, 110-114.	1.2	3
1735	Micropore Formation of $[\text{Zn}_2(\text{Oxac})(\text{Taz})_2] \cdot (\text{H}_2\text{O})_{2.5}$ via CO_2 Adsorption. Langmuir, 2017, 33, 680-684.	1.6	2
1736	In situ identification of kinetic factors that expedite inorganic crystal formation and discovery. Journal of Materials Chemistry C, 2017, 5, 5709-5717.	2.7	30
1737	Ultraviolet saturable absorption and ultrafast carrier dynamics in ultrasmall black phosphorus quantum dots. Nanoscale, 2017, 9, 4683-4690.	2.8	98
1738	First-principles investigation of structural and magnetic disorder in CuNiMnAl and CuNiMnSn Heusler alloys. Physical Review B, 2017, 95, .	1.1	6
1739	Elementary steps in acetone condensation reactions catalyzed by aluminosilicates with diverse void structures. Journal of Catalysis, 2017, 346, 134-153.	3.1	73
1740	Understanding the Structural and Electronic Effect of Zr^{4+} -Doped $\text{KNb}(\text{Zr})\text{O}_3$ Perovskite for Enhanced Photoactivity: A Combined Experimental and Computational Study. Journal of Physical Chemistry C, 2017, 121, 2597-2604.	1.5	9

#	ARTICLE	IF	CITATIONS
1741	Low Voltage Sodium Intercalation in $\text{Na}_x\text{V}_x\text{Ti}_{1-x}\text{O}_2$ ($2/3 \leq x \leq 1$). Journal of the Electrochemical Society, 2017, 164, A490-A497.	1.3	8
1742	Intrinsic Superhydrophilicity of Titania-Terminated Surfaces. Journal of Physical Chemistry C, 2017, 121, 2268-2275.	1.5	19
1743	Magnetism and magnetocrystalline anisotropy in vacancy doped and (non)metal adsorbed single-layer PtSe_2 . Computational Materials Science, 2017, 129, 171-177.	1.4	14
1744	Tuning Electronic Properties and Band Alignments of Phosphorene Combined With MoSe_2 and WSe_2 . Journal of Physical Chemistry C, 2017, 121, 3862-3869.	1.5	55
1745	The "electron crystal" behavior in copper chalcogenides Cu_2X (X = Se, S). Journal of Materials Chemistry A, 2017, 5, 5098-5105.	5.2	81
1746	Novel environment-friendly yellow pigments based on praseodymium(III) tungstate. Ceramics International, 2017, 43, 7366-7368.	2.3	23
1747	Investigation of CeTi_2O_6 - and $\text{CaZrTi}_2\text{O}_7$ -containing glass-ceramic composite materials. Canadian Journal of Chemistry, 2017, 95, 1110-1121.	0.6	13
1748	Hydrothermal Synthesis, Structure, and Superconductivity of Simple Cubic Perovskite $(\text{Ba}_{0.62}\text{K}_{0.38})(\text{Bi}_{0.92}\text{Mg}_{0.08})\text{O}_3$ with $T_c \approx 30$ K. Inorganic Chemistry, 2017, 56, 3174-3181.	1.9	26
1749	Equilibrium crystal shape of BaZrO_3 and space charge formation in the (011) surface by using ab-initio thermodynamics. Journal of the Korean Physical Society, 2017, 70, 75-80.	0.3	6
1750	A DFT+U investigation of hydrogen adsorption on the LaFeO_3 (010) surface. Physical Chemistry Chemical Physics, 2017, 19, 7399-7409.	1.3	28
1751	Screening for Cu-S based thermoelectric materials using crystal structure features. Journal of Materials Chemistry A, 2017, 5, 5013-5019.	5.2	47
1752	Synthesis, crystal structure, and magnetic properties of $\text{Ba}_3\text{Os}_2\text{O}_9$: A new osmate with $\text{Cs}_3\text{Ti}_2\text{Cl}_9$ -type structure. Journal of Solid State Chemistry, 2017, 249, 15-20.	1.4	4
1753	Structural evolution, growth mechanism and photoluminescence properties of CuWO_4 nanocrystals. Ultrasonics Sonochemistry, 2017, 38, 256-270.	3.8	60
1754	Structure and Charge Density Properties of $(1-x)(\text{Na}_y\text{K}_y\text{NbO}_3)_x\text{BaTiO}_3$ Lead-Free Ceramic Solid Solution. Journal of Electronic Materials, 2017, 46, 4187-4196.	1.0	2
1755	A-Site and B-Site Charge Orderings in an d Level Controlled Perovskite Oxide PbCoO_3 . Journal of the American Chemical Society, 2017, 139, 4574-4581.	6.6	52
1756	$\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \langle \text{mml:mi} \text{BaSn} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \langle \text{mml:mi} \rangle \text{ : A wide-gap strong topological insulator. Physical Review B, 2017, 95, .$		
1757	Evolution of Eu valence and superconductivity in layered $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \langle \text{mml:msub} \langle \text{mml:mi} \rangle \text{Eu} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \langle \text{mml:mn} \rangle 0.5 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \langle \text{mml:mi} \rangle \text{ system. Physical Review B, 2017, 95, .$		
1758	^{31}P -dephased, ^{13}C -detected REDOR for NMR crystallography at natural isotopic abundance. Journal of Magnetic Resonance, 2017, 278, 8-17.	1.2	8

#	ARTICLE	IF	CITATIONS
1759	Ag ^I and Pb ^{II} as Additional Assembling Cations in Uranyl Coordination Polymers and Frameworks. <i>Crystal Growth and Design</i> , 2017, 17, 2116-2130.	1.4	39
1760	Magnetic glass state and magnetoresistance in SrLaFeCoO ₆ double perovskite. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 095801.	0.7	10
1761	Defect induced phonon scattering for tuning the lattice thermal conductivity of SiO ₂ thin films. <i>AIP Advances</i> , 2017, 7, 015038.	0.6	6
1762	Structural and compositional variations of basic Cu(II) chlorides in the herbertsmithite and gillardite structure field. <i>Mineralogical Magazine</i> , 2017, 81, 123-134.	0.6	3
1763	Structural Evolution and Atom Clustering in $\hat{\Gamma}^2$ -SiAlON: $\hat{\Gamma}^2$ -Si ₆ Al _z O _z N ₈ . <i>Inorganic Chemistry</i> , 2017, 56, 2153-2158.	1.9	24
1764	Effect of samarium and vanadium co-doping on structure, ferroelectric and photocatalytic properties of bismuth titanate. <i>RSC Advances</i> , 2017, 7, 9680-9692.	1.7	39
1765	High temperature ferromagnetism in π -conjugated two-dimensional metal-organic frameworks. <i>Chemical Science</i> , 2017, 8, 2859-2867.	3.7	86
1766	Hydrogen weakens interlayer bonding in layered transition metal sulfide Fe _{1+x} S. <i>Journal of Materials Chemistry A</i> , 2017, 5, 5030-5035.	5.2	11
1767	First-principles calculations of Mg _{1-x} Cu _x SiP ₂ alloys with x=0.0, 0.25, 0.5, 0.75 and 1.0. <i>Journal of Alloys and Compounds</i> , 2017, 705, 211-217.	2.8	7
1768	Effects of interlayer polarization field on the band structures of the WS ₂ /MoS ₂ and WSe ₂ /MoSe ₂ heterostructures. <i>Surface Science</i> , 2017, 661, 1-9.	0.8	7
1769	Solute Effect on Strength and Formability of Mg: A First-Principle Study. <i>Minerals, Metals and Materials Series</i> , 2017, , 483-489.	0.3	3
1770	Magnetic interactions in rhenium-containing rare earth double perovskites Sr ₂ LnReO ₆ (Ln=rare). <i>Tj ETQq1 1 0.784314 rgBT/Overlo</i>	1.4	11
1771	A zero-thermal-quenching phosphor. <i>Nature Materials</i> , 2017, 16, 543-550.	13.3	748
1772	Magnetic Properties of CeMn ₂ Co _x Ge ₄ O ₁₂ (0 ≤ x ≤ 2) as a Function of Temperature and Magnetic Field. <i>Inorganic Chemistry</i> , 2017, 56, 2750-2762.		8
1773	Charge transfer induced polymerization of EDOT confined between 2D titanium carbide layers. <i>Journal of Materials Chemistry A</i> , 2017, 5, 5260-5265.	5.2	142
1774	Tetrahedral and Cuboidal Clusters in Complexes of Uranyl and Alkali or Alkaline-Earth Metal Ions with <i>rac</i> - and (<i>1R</i> , <i>2R</i>)- <i>trans</i> -1,2-Cyclohexanedicarboxylate. <i>Crystal Growth and Design</i> , 2017, 17, 2881-2892.	1.4	28
1775	Synthesis and luminescence properties of La _{0.67} Mg _{0.5} W _{0.5} O ₃ :Tb ³⁺ green phosphors. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 9798-9803.	1.1	2
1776	Synthesis, characterization and phosphatase inhibitory activity of dioxidovanadium(V) complexes with Schiff base ligands derived from pyridoxal and resorcinol. <i>Polyhedron</i> , 2017, 130, 184-194.	1.0	13

#	ARTICLE	IF	CITATIONS
1777	Electronic structure and chemical bonding in La _{1-x} Sr _x MnO ₃ perovskite ceramics. <i>Materials Research Express</i> , 2017, 4, 046103.	0.8	11
1778	111-Type Semiconductor ReGaSi Follows 14 π Rules. <i>Inorganic Chemistry</i> , 2017, 56, 5165-5172.	1.9	10
1779	Proton conduction across and along BaO π and ZrO 2π -terminated (001) BaZrO ₃ surfaces using density functional theory. <i>Solid State Ionics</i> , 2017, 306, 137-141.	1.3	7
1780	Uranyl Complexes as Scaffolding or Spacers for Cucurbit[6]uril Molecules in Homo π -and Heterometallic Species, Including a Uranyl π -Lanthanide Complex. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2876-2882.	1.0	10
1781	The Role of Structural and Compositional Heterogeneities in the Insulator-to-Metal Transition in Hole-Doped APd ₃ O ₄ (A = Ca, Sr). <i>Inorganic Chemistry</i> , 2017, 56, 5158-5164.	1.9	8
1782	Experimental and computational study of the magnetic properties of ZrMn 2π CoxGe ₄ O ₁₂ . <i>Dalton Transactions</i> , 2017, 46, 6921-6933.	1.6	7
1783	Enhanced atomic oxygen adsorption on defective nickel surfaces: An ab initio study. <i>Surface Science</i> , 2017, 663, 62-70.	0.8	5
1784	First-principle studies of radioactive fission products Cs/Sr/Ag/I adsorption on chrome π -molybdenum steel in Chinese 200MW HTR-PM. <i>Nuclear Science and Techniques/Hewuli</i> , 2017, 28, 1.	1.3	3
1785	Studies on phase transition temperature of rare earth niobates Ln ₃ NbO ₇ (Ln = Pr, Sm, Eu) with orthorhombic fluorite-related structure. <i>Solid State Sciences</i> , 2017, 68, 19-24.	1.5	7
1786	Effective Passivation and Tunneling Hybrid a-SiO _x (In) Layer in ITO/n-Si Heterojunction Photovoltaic Device. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 17565-17575.	4.0	16
1787	Crystal growth and stoichiometry-dependent properties of the ferromagnetic Weyl semimetal ZrCo 2π Sn. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 225702.	0.7	7
1788	Charge optimized many body (COMB) potentials for Pt and Au. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 225901.	0.7	12
1789	Investigating phase formations in cast AlFeCoNiCu high entropy alloys by combination of computational modeling and experiments. <i>Materials and Design</i> , 2017, 127, 224-232.	3.3	35
1790	Yellow MgV ₂ O ₆ ·2H ₂ O nanophosphor synthesized by a water-assisted solid-state reaction (WASSR) method at low temperature below 80 π C. <i>Dyes and Pigments</i> , 2017, 145, 339-344.	2.0	3
1791	Enhancing Dissociative Adsorption of Water on Cu(111) via Chemisorbed Oxygen. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12117-12126.	1.5	17
1792	Systematic Investigation into Mg ²⁺ /Li ⁺ Dual-Cation Transport in Chevrel Phases Using Computational and Experimental Approaches. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12617-12623.	1.5	14
1793	Theoretical perspectives on the structure, electronic, and optical properties of titanosilicates Li ₂ M ₄ [(TiO)Si ₄ O ₁₂] (M = K ⁺), Tj ETQq0 0 0 rgBT1/0verlock010 Tf 50 9		
1794	Bi Substitution Effects on Superconductivity of Valence-Skip Superconductor AgSnSe ₂ . <i>Journal of the Physical Society of Japan</i> , 2017, 86, 054711.	0.7	3

#	ARTICLE	IF	CITATIONS
1795	Effects of on-site Coulomb interaction (<i>U</i>) on the structural and electronic properties of half-metallic ferromagnetic orthorhombic $\text{Pr}_{0.75}\text{Na}_{0.25}\text{MnO}_3$ manganite: a LDA+ <i>U</i> calculation and experimental study. <i>Materials Research Express</i> , 2017, 4, 066103.	0.8	10
1796	Influence of Electrolyte Cations on Ni(Fe)OOH Catalyzed Oxygen Evolution Reaction. <i>Chemistry of Materials</i> , 2017, 29, 4761-4767.	3.2	105
1797	Prediction of <i>T_c</i> and <i>H_{c2}</i> Phase Two-Dimensional Transition-Metal Carbides/Nitrides and Their Semiconducting-Metallic Phase Transition. <i>ChemPhysChem</i> , 2017, 18, 1897-1902.	1.0	30
1798	Synthesis of novel hydride $\text{Li}_3\text{AlFeH}_8$ at high temperature and pressure. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 22489-22495.	3.8	8
1799	Thermally Stable Sr_2RuO_4 Electrode for Oxide Heterostructures. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 21314-21321.	4.0	17
1800	<i>In Situ</i> Neutron Diffraction Studies of the Ion Exchange Synthesis Mechanism of $\text{Li}_2\text{Mg}_2\text{P}_3\text{O}_9\text{N}$: Evidence for a Hidden Phase Transition. <i>Journal of the American Chemical Society</i> , 2017, 139, 9192-9202.	6.6	19
1801	Crystal Structures of CaB_3N_3 at High Pressures. <i>Inorganic Chemistry</i> , 2017, 56, 7449-7453.	1.9	2
1802	First-principles study of the structural stability and electrochemical properties of Na_2MSiO_4 (M = Mn, Fe, Co and Ni) polymorphs. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14462-14470.	1.3	31
1803	Low-Overpotential Electroreduction of Carbon Monoxide Using Copper Nanowires. <i>ACS Catalysis</i> , 2017, 7, 4467-4472.	5.5	137
1804	Atomic structure of the Fe/Fe ₃ C interface with the Isaichev orientation in pearlite. <i>Philosophical Magazine</i> , 2017, 97, 2375-2386.	0.7	22
1805	Synthesis, structure and photocatalytic activity of layered LaOInS_2 . <i>Journal of Materials Chemistry A</i> , 2017, 5, 14270-14277.	5.2	30
1806	Effect of aliovalent dopants on the kinetics of spinodal decomposition in rutile-type TiO_2 -VO ₂ . <i>Journal of the European Ceramic Society</i> , 2017, 37, 3177-3183.	2.8	8
1807	Synthesis of $\text{Sr}_2\text{Si}_5\text{N}_8\text{:Ce}^{3+}$ phosphors for white LEDs via efficient chemical vapor deposition. <i>Scientific Reports</i> , 2017, 7, 45832.	1.6	7
1808	Synthesis, characterization and catalytic properties of a copper-containing polyoxovanadate nanocluster in azide-alkyne cycloaddition. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1564-1572.	0.8	9
1809	Crystal Structure and Bonding Analysis of $(\text{La}_{0.8}\text{Ca}_{0.2})(\text{Cr}_{0.9}\text{Co}_{0.1}\text{Cu}_x)\text{O}_3$ Ceramics. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2017, 72, 383-395.	0.7	1
1810	Investigation of the shear response and geometrically necessary dislocation densities in shear localization in high-purity titanium. <i>International Journal of Plasticity</i> , 2017, 92, 148-163.	4.1	31
1811	Lithiation-enhanced charge transfer and sliding strength at the silicon-graphene interface: A first-principles study. <i>Acta Mechanica Sinica</i> , 2017, 30, 254-262.	1.0	9
1812	Magnetic interactions in praseodymium ruthenate Pr_3RuO_7 with fluorite-related structure. <i>Journal of Solid State Chemistry</i> , 2017, 250, 100-106.	1.4	7

#	ARTICLE	IF	CITATIONS
1813	Synthesis and photoluminescent characteristics of Eu 3+ -doped M ₂ MoO ₄ (M=Sr, Ba) nanophosphors by a hydrothermal method. <i>Journal of Rare Earths</i> , 2017, 35, 347-3355.	2.5	15
1814	Concentration effect on equilibrium fractionation of Mg-Ca isotopes in carbonate minerals: Insights from first-principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2017, 208, 185-197.	1.6	72
1815	Magnetic states of MnP: muon-spin rotation studies. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 164003.	0.7	11
1816	Linker Functionalization in MIL-47(V)-R Metal-Organic Frameworks: Understanding the Electronic Structure. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8014-8022.	1.5	10
1817	Embedded atom method interatomic potentials fitted upon density functional theory calculations for the simulation of binary Pt Ni nanoparticles. <i>Computational Materials Science</i> , 2017, 133, 185-193.	1.4	4
1818	Structural, Magnetic, Optical, and MEM Studies on Co-precipitated X _{0.4} Zn _{0.6} Fe ₂ O ₄ (X = Co, Mn) Nanoferrite Particles. <i>Journal of Superconductivity and Novel Magnetism</i> , 2017, 30, 2673-2682.	0.8	4
1819	Enhancement of tetragonal anisotropy and stabilisation of the tetragonal phase by Bi/Mn-double-doping in BaTiO ₃ ferroelectric ceramics. <i>Scientific Reports</i> , 2017, 7, 45842.	1.6	21
1820	Electronic structure and bonding interactions in Ba _{1-x} Sr _x Zr _{0.1} Ti _{0.9} O ₃ ceramics. <i>Frontiers of Materials Science</i> , 2017, 11, 182-189.	1.1	5
1821	Occupation deficiency in layered structures of UNi _x Sb ₂ (0 ≤ x ≤ 1) studied by density functional theory supercell calculations. <i>Computational Materials Science</i> , 2017, 134, 166-170.	1.4	0
1822	Counterintuitive Adsorption of [PW ₁₁ O ₃₉] ⁷⁻ on Au(100). <i>Inorganic Chemistry</i> , 2017, 56, 3961-3969.	1.9	18
1823	Size dependent tunnel diode effects in gold tipped CdSe nanodumbbells. <i>Journal of Chemical Physics</i> , 2017, 146, 054703.	1.2	1
1824	Stacking fault energies of nondilute binary alloys using special quasirandom structures. <i>Physical Review B</i> , 2017, 95, .	1.1	9
1825	Interfacial structures and energetics of the strengthening precipitate phase in creep-resistant Mg-Nd-based alloys. <i>Scientific Reports</i> , 2017, 7, 40540.	1.6	9
1826	Pentavalent uranium complex oxides: A case study on double perovskites Ba ₂ REU ₅ O ₁₆ (RE=La, Nd, Sm). <i>Journal of Alloys and Compounds</i> , 2017, 708, 1168-1177.	2.8	3
1827	Using Similarity Metrics to Quantify Differences in High-Throughput Data Sets: Application to X-ray Diffraction Patterns. <i>ACS Combinatorial Science</i> , 2017, 19, 25-36.	3.8	20
1828	Photoelectrochemical Properties and Behavior of Bi-SnWO ₄ Photoanodes Synthesized by Hydrothermal Conversion of WO ₃ Films. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 1459-1470.	4.0	42
1829	On the character of the optical transitions in closed-shell transition metal oxides doped with Bi ³⁺ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2591-2596.	1.3	27
1830	Discovery of novel inorganic Mn ⁵⁺ -doped sky-blue pigments based on Ca ₆ BaP ₄ O ₁₇ : Crystal structure, optical and color properties, and color durability. <i>Dyes and Pigments</i> , 2017, 139, 344-348.	2.0	29

#	ARTICLE	IF	CITATIONS
1831	In Situ Reversible Ionic Control for Nonvolatile Magnetic Phases in a Donor/Acceptor Metal-Organic Framework. <i>Advanced Functional Materials</i> , 2017, 27, 1604990.	7.8	27
1832	Stabilized Octahedral Frameworks in Layered Double Hydroxides by Solid-Solution Mixing of Transition Metals. <i>Advanced Functional Materials</i> , 2017, 27, 1605225.	7.8	58
1833	Thermoelectric Properties of Na ₂ ZnSn ₅ Dimorphs with Na Atoms Disordered in Tunnels. <i>Chemistry of Materials</i> , 2017, 29, 859-866.	3.2	5
1834	¹¹ B NMR Study of WB ₂ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 1315-1320.	1.5	4
1835	Complexation of Uranyl Ion with Sulfonates: One- to Three-Dimensional Assemblies with 1,5- and 2,7-Naphthalenedisulfonates. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 979-987.	1.0	11
1836	The first study of antiferromagnetic eosphorite-childrenite series (Mn _{1-x} Fe _x)AlP(OH)2H ₂ O (x=0.5). <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 428, 17-27.	1.0	4
1837	First-principles calculations on the structural and electronic properties of cubic KCaF ₃ and NaCaF ₃ (001) surfaces. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 890-895.	0.9	11
1838	Crystal structure and bonding characteristics of transformation products of bcc Fe ² in Ti-Mo alloys. <i>Journal of Alloys and Compounds</i> , 2017, 705, 769-781.	2.8	25
1839	Theoretical study of deposition-induced point defects in ZnO. <i>Surface and Coatings Technology</i> , 2017, 309, 531-535.	2.2	3
1840	Intrinsic Phase Diagram of Superconductivity in the BiCh ₂ -Based System Without In-Plane Disorder. <i>Journal of the Physical Society of Japan</i> , 2017, 86, 074701.	0.7	35
1841	Encapsulating Iodine and Copper into Copper(I) Clusters Stabilized by Dichalcogenolate Ligands: Stability, Structure, and Optical Properties. <i>Inorganic Chemistry</i> , 2017, 56, 14135-14146.	1.9	12
1842	Enhancing the solar energy conversion efficiency of solution-deposited Bi ₂ S ₃ thin films by annealing in sulfur vapor at elevated temperature. <i>Sustainable Energy and Fuels</i> , 2017, 1, 2134-2144.	2.5	25
1843	A correlative experimental and ab initio approach to improve the fracture behavior of Mo thin films by alloying with Cu. <i>Applied Physics Letters</i> , 2017, 111, 134101.	1.5	5
1844	Predicting displacements of octahedral cations in ferroelectric perovskites using machine learning. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 962-967.	0.5	21
1845	Synthesis and crystal structure of Ca(Co,Mg)Si ₂ O ₆ pyroxenes: effect of the cation substitution on cell volume. <i>Mineralogical Magazine</i> , 2017, 81, 1129-1139.	0.6	5
1846	Remarkably Strong Chemisorption of Nitric Oxide on Insulating Oxide Films Promoted by Hybrid Structure. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21482-21490.	1.5	10
1847	Crystal structure and photoluminescent property of Eu ³⁺ -doped K ₃ GdSi ₂ O ₇ . <i>Journal of Asian Ceramic Societies</i> , 2017, 5, 377-380.	1.0	8
1848	K _{1+2x} Ni _{1-x} Fe ₂ (AsO ₄) ₃ (x=) Tj ETQq1 1 0.7843 Crystallographic Communications, 2017, 73, 239-245.	0.2	2

#	ARTICLE	IF	CITATIONS
1849	High-temperature synthesis and electronic bonding analysis of Ca-doped LaMnO ₃ rare-earth manganites. <i>Rare Metals</i> , 2022, 41, 3932-3942.	3.6	4
1850	Pressure tuning of bond-directional exchange interactions and magnetic frustration in the hyperhoneycomb iridate $\text{Yb}_2\text{Ir}_2\text{O}_7$. <i>Physical Review B</i> , 2017, 96, .	1.1	47
1851	Experimental and theoretical exploration of mechanical stability of Pt/NbO ₂ interfaces for thermoelectric applications. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 455502.	1.3	4
1852	Metastable Stacking-Polymorphism in Ge ₂ Sb ₂ Te ₅ . <i>Inorganic Chemistry</i> , 2017, 56, 11990-11997.	1.9	16
1853	The electronic structure of Ag _{1-x} Sn _{1+x} Se ₂ (x = 0.0, 0.1, 0.2, 0.25 and 1.0). <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26672-26678.	1.3	19
1854	Crystal structure, site selectivity, and electronic structure of layered chalcogenide LaOBiPbS ₃ . <i>Europhysics Letters</i> , 2017, 119, 26002.	0.7	20
1855	Grand canonical Monte Carlo simulation study of cyclohexane, oxane, 1,4-dioxane, and 1,3,5-trioxane confined in carbon slit pore. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2017, 533, 255-266.	2.3	2
1856	Structural Consequences of 1,4-Cyclohexanedicarboxylate Cis/Trans Isomerism in Uranyl Ion Complexes: From Molecular Species to 2D and 3D Entangled Nets. <i>Inorganic Chemistry</i> , 2017, 56, 13464-13481.	1.9	54
1857	Computational and Experimental Investigation of the Electrochemical Stability and Li-Ion Conduction Mechanism of LiZr ₂ (PO ₄) ₃ . <i>Chemistry of Materials</i> , 2017, 29, 8983-8991.	3.2	68
1858	Evidence for antiferromagnetic-type ordering off-electron multipoles in PrIr ₂ Zn ₂₀ . <i>Physical Review B</i> , 2017, 95, .	1.1	22
1859	Hydrothermal Preparation, Crystal Chemistry, and Redox Properties of Iron Muscovite Clay. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 34024-34032.	4.0	5
1860	Synthesis and investigation of neptunium zirconium phosphate, a member of the NZP family: crystal structure, thermal behaviour and Mössbauer spectroscopy studies. <i>Dalton Transactions</i> , 2017, 46, 11626-11635.	1.6	15
1861	Barium Sulfide under Pressure: Discovery of Metastable Polymorphs and Investigation of Electronic Properties on ab Initio Level. <i>Inorganic Chemistry</i> , 2017, 56, 10644-10654.	1.9	20
1862	The adsorption of Cu on the CeO ₂ (110) surface. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27191-27203.	1.3	17
1863	Finding and characterization of an energetically favorable cubic Ce _{0.75} Zr _{0.25} O ₂ solid solution using genetic algorithm and density functional theory. <i>Computational Materials Science</i> , 2017, 138, 219-224.	1.4	5
1864	Unusual, broad red emission of novel Ce ³⁺ -activated Sr ₃ Sc ₄ O ₉ phosphors under visible-light excitation. <i>Journal of Materials Chemistry C</i> , 2017, 5, 9472-9478.	2.7	67
1865	Scaling reducibility of metal oxides. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	67
1866	Electronic and optical properties of the wurtzite-ZnO/CH ₃ NH ₃ PbI ₃ interface: first-principles calculations. <i>Journal of Materials Science</i> , 2017, 52, 13841-13851.	1.7	10

#	ARTICLE	IF	CITATIONS
1885	The relationship between atomic structure and magnetic property of amorphous Fe ₇₈ Si ₉ B ₁₃ alloy at different pressures. Journal of Magnetism and Magnetic Materials, 2017, 443, 216-221.	1.0	15
1886	Synthesis of rutile-type solid solution Ni _{1-x} Co _x Ti(Nb _{1-y} Ta _y) ₂ O ₈ (O ^Δ x Δ ^Δ 1, O ^Δ y Δ ^Δ 1) and its optical property. Journal of Asian Ceramic Societies, 2017, 5, 284-289.	1.0	14
1887	EDTA-assisted phase conversion synthesis of (Gd _{0.95} RE _{0.05})PO ₄ nanowires (RE = Eu, Tb) and investigation of photoluminescence. Science and Technology of Advanced Materials, 2017, 18, 447-457.	2.8	10
1888	Rich magnetoelectric phase diagrams of multiferroic single-crystal $\hat{\pm}^{\sim}$ NaFeO ₂ . Physical Review B, 2017, 96, .	1.1	5
1889	Structural chemistry and magnetic properties of Ln MnFeGe ₄ O ₁₂ (Ln = Y, Eu, Lu). Journal of Solid State Chemistry, 2017, 254, 40-46.	1.4	4
1890	Stabilization of novel high temperature phase yellow-emitting \hat{f} -type (Ba _{1-x} Y _x Eu _x Mg _y) ₂ P ₂ O ₇ phosphors using a melt synthesis technique. Inorganic Chemistry Frontiers, 2017, 4, 1562-1567.	3.0	7
1891	Potentiality of delocalized states in indium-involved amorphous silicon oxide. Applied Physics Letters, 2017, 110, 213902.	1.5	9
1892	Carbonate substitution in the mineral component of bone: Discriminating the structural changes, simultaneously imposed by carbonate in A and B sites of apatite. Journal of Solid State Chemistry, 2017, 255, 27-35.	1.4	198
1893	Growth mechanism of ceria nanorods by precipitation at room temperature and morphology-dependent photocatalytic performance. CrystEngComm, 2017, 19, 4766-4776.	1.3	34
1894	Pressure-induced anomalous valence crossover in cubic YbCu ₅ -based compounds. Scientific Reports, 2017, 7, 5846.	1.6	14
1895	Magnetic properties of the CrMnFeCoNi high-entropy alloy. Physical Review B, 2017, 96, .	1.1	124
1896	Luminescence properties of the NaLaMg _{0.92} Ca _{0.08} WO ₆ :Sm ³⁺ red phosphor. Journal of Materials Science: Materials in Electronics, 2017, 28, 16755-16761.	1.1	4
1897	The magnetic state of $\hat{\eta}$ -Fe ₂ N. AIP Conference Proceedings, 2017, , .	0.3	0
1898	Structure prediction of aluminum nitride combining data mining and quantum mechanics. CrystEngComm, 2017, 19, 5259-5268.	1.3	31
1899	Correlation between optical properties and environmental parameter of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{ZnWO} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 4 \langle \text{mml:mn} \rangle \langle \text{mml:mn} \rangle$ ceramic using complex chemical bond theory. Journal of Alloys and Compounds, 2017, 726, 1014-1023.	2.8	21
1900	Van der Waals Interactions and Anharmonicity in the Lattice Vibrations, Dielectric Constants, Effective Charges, and Infrared Spectra of the Organic Inorganic Halide Perovskite CH ₃ NH ₃ PbI ₃ . Journal of Physical Chemistry C, 2017, 121, 18459-18471.	1.5	24
1901	Diffusion quantum Monte Carlo calculations of SrFeO ₃ and LaFeO ₃ . Journal of Chemical Physics, 2017, 147, 034701.	1.2	27
1902	Single crystal growth of \hat{f}^2 -Tb ₂ (MoO ₄) ₃ and its evaluation. Ferroelectrics, 2017, 511, 82-87.	0.3	1

#	ARTICLE	IF	CITATIONS
1903	Modulating the properties of monolayer C ₂ N: A promising metal-free photocatalyst for water splitting. Chinese Physics B, 2017, 26, 087301.	0.7	12
1904	Lead(ii): Lewis acid and occasional base, as illustrated by its complex with 1,5-naphthalenedisulfonate and 5-methyl-1,10-phenanthroline. Dalton Transactions, 2017, 46, 11533-11536.	1.6	7
1905	Effect of oxygen vacancy segregation in Au or Pt/oxide hetero-interfaces on electronic structures. RSC Advances, 2017, 7, 36034-36037.	1.7	2
1906	Crystal structures, magnetic properties, and DFT calculation of B-site defected 12L-perovskites Ba ₂ La ₂ MW ₂ O ₁₂ (M = Mn, Co, Ni, Zn). Journal of Physics Condensed Matter, 2017, 29, 365802.		
1907	Wettability alteration of calcite oil wells: Influence of smart water ions. Scientific Reports, 2017, 7, 17365.	1.6	25
1908	Tuning the metamagnetism in a metallic helical antiferromagnet. Applied Physics Letters, 2017, 111, 232404.	1.5	4
1909	Synthesis, Crystal Structure, and Physical Properties of New Layered Oxychalcogenide La ₂ O ₂ Bi ₃ AgS ₆ . Journal of the Physical Society of Japan, 2017, 86, 124802.	0.7	18
1910	Lithium diffusion study in Li ₂ MnO ₃ and Li _{1.17} Ni _{0.17} Mn _{0.67} O ₂ : a combined experimental and computational approach. Physical Chemistry Chemical Physics, 2017, 19, 31724-31730.	1.3	15
1911	SnAs-Based Layered Superconductor NaSn ₂ As ₂ . Journal of the Physical Society of Japan, 2017, 86, 123701.	0.7	33
1912	Large exchange anisotropy in quasi-one-dimensional spin-fluoride antiferromagnets with a ground state. Physical Review B, 2017, 96, 114407.	1.1	15
1913	Lattice response of the porous coordination framework Zn(hba) to guest adsorption. Powder Diffraction, 2017, 32, S49-S53.	0.4	1
1914	Thermal Equation of State of Natural Ti-Bearing Clinohumite. Journal of Geophysical Research: Solid Earth, 2017, 122, 8943-8951.	1.4	12
1915	Mechanistic Insights for Low-Overpotential Electroreduction of CO ₂ to CO on Copper Nanowires. ACS Catalysis, 2017, 7, 8578-8587.	5.5	106
1916	Phase equilibria in the ZrO ₂ -YO _{1.5} -TaO _{2.5} system at 1500 Å°C. Journal of the European Ceramic Society, 2017, 37, 4888-4901.	2.8	55
1917	Structure Prediction for Surface-Induced Phases of Organic Monolayers: Overcoming the Combinatorial Bottleneck. Nano Letters, 2017, 17, 4453-4460.	4.5	26
1918	Inducement of ferromagnetic-metallic phase in intermediate-doped charge-ordered Pr _{0.75} Na _{0.25} MnO ₃ manganite by K ⁺ substitution. Physica B: Condensed Matter, 2017, 521, 281-294.	1.3	18
1919	Speciation of magnesium in monohydrocalcite: XANES, ab initio and geochemical modeling. Geochimica Et Cosmochimica Acta, 2017, 213, 457-474.	1.6	19
1920	Generalized stacking fault energies, ductilities, and twinnabilities of CoCrFeNi-based face-centered cubic high entropy alloys. Scripta Materialia, 2017, 139, 83-86.	2.6	129

#	Superc	IF	CITATIONS
1921	Superconductivity in a new intermetallic structure type based on endohedral $\text{Ta}@$ Ir_7Ge_4 Spatially Confined Li-Oxygen Interaction in the Tunnel of Li-MnO_2 Catalyst for Air Battery: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 16193-16200.	1.1	16
1922	First-principles description of van der Waals bonded spin-polarized systems using the vdW-DF+ method: Application to solid oxygen at low pressure. Physical Review B, 2017, 95, .	1.5	15
1923	Photon and electron beam pumped luminescence of Ho^{3+} activated CaMoO_4 phosphor. Applied Surface Science, 2017, 423, 1169-1175.	1.1	6
1924	Effect of A mixing on elastic modulus, cleavage stress, and shear stress in the $\text{mrow} < \text{msub} < \text{mi}$	3.1	17
1925			

#	ARTICLE	IF	CITATIONS
1939	First-principles study on the adhesive properties of Al/TiC interfaces: Revisited. Computational Materials Science, 2017, 126, 108-120.	1.4	23
1940	Hydrothermal synthesis and crystal structure of a new lithium copper bismuth oxide, LiCuBiO ₄ . Journal of Solid State Chemistry, 2017, 245, 30-33.	1.4	7
1941	Structural and luminescence responses of CaMoO ₄ nano phosphors synthesized by hydrothermal route to swift heavy ion irradiation: Elemental and spectral stability. Acta Materialia, 2017, 124, 109-119.	3.8	26
1942	Effect of Ce addition on the electronic structure and bonding in BaTi _{1-x} Ce _x O ₃ ceramics. Journal of Materials Science: Materials in Electronics, 2017, 28, 2624-2633.	1.1	2
1943	Composition driven structural transition in La ₂ Sr _{1-x} CuRuO ₆ (0 ≤ x ≤ 1) double perovskites. Journal of Alloys and Compounds, 2017, 693, 1096-1101.	2.8	3
1944	Bulk Superconductivity Induced by Se Substitution in BiCh ₂ -Based Layered Compounds Eu _{0.5} Ce _{0.5} FBiS ₂ (x = 2, 3). Journal of the Physical Society of Japan, 2017, 86, 104712.	0.7	13
1945	Tunable electronic and optical properties of gas molecules adsorbed monolayer graphitic ZnO: Implications for gas sensor and environment monitoring. Journal of Applied Physics, 2017, 122, .	1.1	11
1946	Half-Metallic Ferromagnetism in Double Perovskite Ca ₂ CoMoO ₆ Compound: DFT+U Calculations. Spin, 2017, 07, 1750009.	0.6	22
1947	Intrinsic optical conductivity of a $\{C\}_2$ symmetric topological insulator. Semiconductor Science and Technology, 2017, 32, 075013.	1.0	1
1948	Complexes of Uranyl Ions with Aromatic Diene and Tetracarboxylates Involving [Ni(bipy) _n] ²⁺ (n = 2, 3) Counterions. European Journal of Inorganic Chemistry, 2017, 2017, 5451-5460.	1.0	9
1949	Dzyaloshinskii-Moriya interaction in O_3 measured by magnetic circular dichroism in resonant inelastic soft x-ray scattering. Physical Review B, 2017, 96, .	1.1	31
1950	Cooperative oxide-ion conduction in apatite-type lanthanum germanate—A first principles study. Journal of the Ceramic Society of Japan, 2017, 125, 105-111.	0.5	5
1951	Preparation and electrode properties of novel redoxable nanosheets of Mn–Ni oxide with and without vacancy defects. Journal of the Ceramic Society of Japan, 2017, 125, 293-298.	0.5	4
1952	Analysis of CO ₂ absorption reaction of Li ₄ SiO ₄ on the basis of Madelung potential of Li site in crystal structure. Journal of the Ceramic Society of Japan, 2017, 125, 383-386.	0.5	9
1953	Thermal conductivity of thin finite-size \hat{I}^2 -SiC calculated by molecular dynamics combined with quantum correction. , 2017, , .		0
1954	Ab initio study of magnetocrystalline anisotropy, magnetostriction, and Fermi surface of Li ₀ FeNi (tetrataenite). Journal Physics D: Applied Physics, 2017, 50, 495008.	1.3	24
1955	Synthesis and crystal structure of pyrochlore-type silver niobate and tantalate. Journal of the Ceramic Society of Japan, 2017, 125, 776-778.	0.5	6
1956	Temperature dependences of the excess current and pseudogap in high-temperature superconductor Bi ₂ Sr ₂ CaCuO ₉ . , 2017, , .		0

#	ARTICLE	IF	CITATIONS
1957	Tungsten Disilicide (WSi_2): Synthesis, Characterization, and Prediction of New Crystal Structures. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017, 643, 2088-2094.	0.6	17
1958	Roles of d- and f-orbital electrons in the complexation of Eu(III) and Am(III) ions with alkyldithiophosphinic acid and alkylphosphinic acid using scalar-relativistic DFT calculations. <i>Journal of Nuclear and Radiochemical Sciences</i> , 2017, 17, 9-15.	0.7	12
1959	Structural Distortion in MnO_2 Nanosheets and Its Suppression by Cobalt Substitution. <i>Nanomaterials</i> , 2017, 7, 295.	1.9	5
1960	Discovery of BiS_2 -Based Superconductor and Material Design Concept. <i>Condensed Matter</i> , 2017, 2, 6.	0.8	8
1961	Borates' Crystal Structures of Prospective Nonlinear Optical Materials: High Anisotropy of the Thermal Expansion Caused by Anharmonic Atomic Vibrations. <i>Crystals</i> , 2017, 7, 93.	1.0	40
1962	High-Pressure Reactivity of Kr and F_2 Stabilization of Krypton in the +4 Oxidation State. <i>Crystals</i> , 2017, 7, 329.	1.0	4
1963	Interfacial properties of hydrides in $\lambda\text{-Zr}$: a theoretical study. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 415001.	0.7	8
1964	Bonding Study on Trivalent Europium Complexes by Combining Mössbauer Isomer Shifts with Density Functional Calculations. <i>Radioisotopes</i> , 2017, 66, 289-300.	0.1	3
1965	Synchrotron powder X-ray diffraction and structural analysis of $Eu_{0.5}La_{0.5}BiS_2$ and Se . <i>Journal of Physics: Conference Series</i> , 2017, 871, 012007.	0.3	6
1966	Stability and elasticity of metastable solid solutions and superlattices in the $Mo-Ni-Ta$ system: First-principles calculations. <i>Materials and Design</i> , 2018, 144, 310-322.	3.3	29
1967	Determination of Debye temperatures and Lamb-Mössbauer factors for $LnFeO_3$ orthoferrite perovskites ($Ln = La, Nd, Sm, Eu, Gd$). <i>Journal of Physics Condensed Matter</i> , 2018, 30, 105704.	1.5	13
1968	Effect of glycine functionalization of 2D titanium carbide (MXene) on charge storage. <i>Journal of Materials Chemistry A</i> , 2018, 6, 4617-4622.	5.2	103
1969	A comprehensive structural and microstructural investigation of a new iron telluride nano phase. <i>Journal of Materials Chemistry C</i> , 2018, 6, 3047-3057.	2.7	13
1970	On the luminescence of Bi^{3+} pairs in oxidic compounds. <i>Journal of Luminescence</i> , 2018, 197, 228-232.	1.5	38
1971	Magnetic Switching by the In Situ Electrochemical Control of Quasi-Spin-Peierls Singlet States in a Three-Dimensional Spin Lattice Incorporating TTF-CNQ Salts. <i>Chemistry - A European Journal</i> , 2018, 24, 4294-4303.	1.7	12
1972	Origins of the Stokes Shift in PbS Quantum Dots: Impact of Polydispersity, Ligands, and Defects. <i>ACS Nano</i> , 2018, 12, 2838-2845.	7.3	50
1973	Perovskite $ThTa_3$: A large-thermopower topological crystalline insulator. <i>Physical Review B</i> , 2018, 97, .	1.1	17
1974	Evolution of Anisotropic Displacement Parameters and Superconductivity with Chemical Pressure in BiS_2 -Based $RE_{0.5}F_{0.5}BiS_2$ ($RE = La, Ce, Pr, \text{ and } Nd$). <i>Journal of the Physical Society of Japan</i> , 2018, 87, 023704.	0.7	34

#	ARTICLE	IF	CITATIONS
1975	Is SrZn ₂ Sb ₂ a Realistic Candidate for High-Temperature Thermoelectric Applications?. Journal of Physical Chemistry C, 2018, 122, 5317-5324.	1.5	8
1976	Neutron scattering study of yttrium iron garnet. Physical Review B, 2018, 97, .	1.1	19
1977	Correlating Transport and Structural Properties in Li _{1+x} Al _x Ge ₂ (PO ₄) ₃ (LAGP) Prepared from Aqueous Solution. ACS Applied Materials & Interfaces, 2018, 10, 10935-10944.	4.0	75
1978	First-principles investigation of polarization and ion conduction mechanisms in hydroxyapatite. Physical Chemistry Chemical Physics, 2018, 20, 8744-8752.	1.3	20
1979	Atomically thin gallium layers from solid-melt exfoliation. Science Advances, 2018, 4, e1701373.	4.7	157
1980	Enhanced hydrothermal crystallization and color tailorable photoluminescence of hexagonal structured YPO ₄ :Sm/Tb nanorods. CrystEngComm, 2018, 20, 2357-2365.	1.3	12
1981	Intrinsic structural distortion and exchange interactions in SmFe _x Cr _{1-x} O ₃ compounds. RSC Advances, 2018, 8, 8842-8848.	1.7	17
1982	A general representation scheme for crystalline solids based on Voronoi-tessellation real feature values and atomic property data. Science and Technology of Advanced Materials, 2018, 19, 231-242.	2.8	24
1983	Unprecedented rapid synthesis of REPO ₄ monospheres (RE ³⁺ =La-Lu lanthanide and Y) and investigation of multi-color photoluminescence. Chemical Engineering Journal, 2018, 343, 16-27.	6.6	22
1984	Strain-engineering stabilization of BaTiO_3 -based polar metals. Physical Review B, 2018, 97, .	1.1	26
1985	Crystal Structure and Superconductivity of Tetragonal and Monoclinic Ce _{1-x} Pr _x OBS ₂ . Inorganic Chemistry, 2018, 57, 5364-5370.	1.9	14
1986	Elastic properties of long periodic stacking ordered phases in Mg-Gd-Al alloys: A first-principles study. Intermetallics, 2018, 98, 18-27.	1.8	21
1987	Structural and electronic properties of V ₂ O ₅ and their tuning by doping with 3d elements – modelling using the DFT+U method and dispersion correction. Physical Chemistry Chemical Physics, 2018, 20, 13934-13943.	1.3	41
1988	Adsorption of rare earth yttrium and ammonium ions on kaolinite surfaces: a DFT study. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	23
1989	Identifying the tuning key of disproportionation redox reaction in terephthalate: A Li-based anode for sustainable organic batteries. Nano Energy, 2018, 47, 301-308.	8.2	17
1990	Shape-, Size-, and Composition-Controlled Thallium Lead Halide Perovskite Nanowires and Nanocrystals with Tunable Band Gaps. Chemistry of Materials, 2018, 30, 2973-2982.	3.2	28
1991	Interfacial electronic states and self-formed p-n junctions in hydrogenated MoS ₂ /SiC heterostructure. Journal of Materials Chemistry C, 2018, 6, 4523-4530.	2.7	37
1992	A catalytic role of surface silanol groups in CO ₂ capture on the amine-anchored silica support. Physical Chemistry Chemical Physics, 2018, 20, 12149-12156.	1.3	18

#	ARTICLE	IF	CITATIONS
1993	The effect of oxygen vacancies on the properties of polar and nonpolar (001) LaAlO ₃ /SrTiO ₃ heterostructures. <i>Applied Surface Science</i> , 2018, 450, 260-264.	3.1	4
1994	Magnetic Studies on Eu ₃ MO ₇ (M = Nb, Ta, Ir) with Fluorite-related Structure by ¹⁵¹ Eu Mössbauer Spectroscopy and Magnetic Susceptibility Measurements. <i>Journal of Solid State Chemistry</i> , 2018, 262, 224-228.	1.4	3
1995	Simulation of defect formation, amorphization and cluster formation processes in nc-TiN/a-Si ₃ N ₄ nanocomposite under Xe irradiation. <i>Computational Materials Science</i> , 2018, 143, 143-156.	1.4	4
1996	Anisotropic Thermal and Guest-Induced Responses of an Ultramicroporous Framework with Rigid Linkers. <i>Chemistry - A European Journal</i> , 2018, 24, 4774-4779.	1.7	3
1997	Tuning of physical properties of Fe ₇ (PO ₄) ₆ by sodium intercalation. <i>Journal of Alloys and Compounds</i> , 2018, 744, 600-605.	2.8	5
1998	The electronic properties of Au clusters on CeO ₂ (110) surface with and without O-defects. <i>Faraday Discussions</i> , 2018, 208, 123-145.	1.6	12
1999	Crystal Growth and Scintillation Properties of Eu ²⁺ doped Cs ₄ CaI ₆ and Cs ₄ SrI ₆ . <i>Journal of Crystal Growth</i> , 2018, 486, 162-168.	0.7	31
2000	Tunable magnetism in the LaAlO ₃ /SrTiO ₃ heterostructure: Insights from first-principles calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 98, 120-124.	1.3	6
2001	Time-Dependent Density Functional Theory Study on Higher Low-Lying Excited States of Au ₂₅ (SR) ₁₈ . <i>Journal of Physical Chemistry C</i> , 2018, 122, 4097-4104.	1.5	17
2002	A spin-orbital-entangled quantum liquid on a honeycomb lattice. <i>Nature</i> , 2018, 554, 341-345.	13.7	276
2003	Effect of Gd substitution on the structural, magnetic, and magnetocaloric properties of HoCrO ₃ . <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	17
2004	An Aqueous Inorganic Polymer Binder for High Performance Lithium-Sulfur Batteries with Flame-Retardant Properties. <i>ACS Central Science</i> , 2018, 4, 260-267.	5.3	147
2005	Chromium removal from aqueous solution by a PEI-silica nanocomposite. <i>Scientific Reports</i> , 2018, 8, 1438.	1.6	101
2006	Polyselenide Anchoring Using Transition-Metal Disulfides for Enhanced Lithium-Selenium Batteries. <i>Inorganic Chemistry</i> , 2018, 57, 2149-2156.	1.9	19
2007	Effect of Te substitution on crystal structure and transport properties of AgBiSe ₂ thermoelectric material. <i>Dalton Transactions</i> , 2018, 47, 2575-2580.	1.6	38
2008	Superconductivity in a New 1144-Type Family of (La,Na)AFe ₄ As ₄ (A = Rb or Cs). <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 868-873.	2.1	19
2009	First-principles study of Cs/Rb co-doped FAPbI ₃ stability and degradation in the presence of water and oxygen. <i>Materials Research Express</i> , 2018, 5, 026203.	0.8	4
2010	Effect of sulphur vacancy and interlayer interaction on the electronic structure and spin splitting of bilayer MoS ₂ . <i>Journal of Physics Condensed Matter</i> , 2018, 30, 125302.	0.7	30

#	ARTICLE	IF	CITATIONS
2011	Lateral Chemical Bonding in Two-Dimensional Transition-Metal Dichalcogenide Metal/Semiconductor Heterostructures. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5401-5410.	1.5	14
2012	Diffusion mechanism in the superionic conductor Li ₄ PS ₄ studied by first-principles calculations. <i>Solid State Ionics</i> , 2018, 319, 83-91.	1.3	23
2013	Mono- and bimetallic nanoparticles decorated KTaO ₃ photocatalysts with improved Vis and UV-Vis light activity. <i>Applied Surface Science</i> , 2018, 441, 993-1011.	3.1	26
2014	Molecular dynamics of the halloysite nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5841-5849.	1.3	39
2015	Correlation between Am(III)/Eu(III) selectivity and covalency in metal-chalcogen bonds using density functional calculations. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2018, 316, 1129-1137.	0.7	17
2016	Roles of Mo Surface Dopants in Enhancing the ORR Performance of Octahedral PtNi Nanoparticles. <i>Nano Letters</i> , 2018, 18, 798-804.	4.5	162
2017	Preparation, electronic structure, and chemical bonding of lead-free (1-x)(K _{0.5} Bi _{0.5})TiO ₃ -xBaTiO ₃ solid solution. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	1.1	2
2018	Ba ₃ CuOs ₂ O ₉ and Ba ₃ ZnOs ₂ O ₉ , a comparative study. <i>Journal of Solid State Chemistry</i> , 2018, 258, 776-780.	1.4	11
2019	Structural controls of CO ₂ on Y, La and Sr incorporation in sodium-rich silicate - carbonate melts by in-situ high P-T EXAFS. <i>Chemical Geology</i> , 2018, 486, 1-15.	1.4	10
2020	Superconductivity on Hole-Doping Side of (La _{0.5-x} Na _{0.5+x})Fe ₂ As ₂ . <i>Journal of the American Chemical Society</i> , 2018, 140, 369-374.	6.6	20
2021	Bluish-White Luminescence in Rare-Earth-Free Vanadate Garnet Phosphors: Structural Characterization of LiCa ₃ MV ₃ O ₁₂ (M = Zn and Mg). <i>Inorganic Chemistry</i> , 2018, 57, 857-866.	1.9	80
2022	Emulating porphyrins with a rippled multivacancy graphene system. <i>Applied Surface Science</i> , 2018, 436, 1173-1180.	3.1	1
2023	NaCl-CsCl structural transition in Sr ₂ PdO ₃ and Sr ₂ TiO ₄ . <i>Journal of Alloys and Compounds</i> , 2018, 737, 230-237.	2.8	1
2024	Efficient cationic agents for exfoliating two-dimensional nickel oxide sheets. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	10
2025	A review of Ga ₂ O ₃ materials, processing, and devices. <i>Applied Physics Reviews</i> , 2018, 5, .	5.5	1,816
2026	Spin density accuracy and distribution in azido Cu(II) complexes: A source function analysis. <i>Journal of Computational Chemistry</i> , 2018, 39, 587-603.	1.5	9
2027	Oxidation behaviour of U ₃ Si ₂ : an experimental and first principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4708-4720.	1.3	23
2028	Experimental and DFT study of the V-Co-Sb ternary system. <i>Journal of Alloys and Compounds</i> , 2018, 739, 771-779.	2.8	5

#	ARTICLE	IF	CITATIONS
2029	Tunable optical properties and stability of lead free all inorganic perovskites ($\text{Cs}_{2-x}\text{Sn}_x\text{Cl}_6$). Journal of Materials Chemistry A, 2018, 6, 2577-2584.	5.2	55
2030	Experimental investigation and simulation of precipitation evolution in Mg-3Nd-0.2Zn alloy. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 60, 58-67.	0.7	17
2031	Origin of High Capacity and Poor Cycling Stability of Li-Rich Layered Oxides: A Long-Duration in Situ Synchrotron Powder Diffraction Study. Chemistry of Materials, 2018, 30, 3656-3667.	3.2	115
2032	Superconductivity in $\text{REO}_{0.5}\text{F}_{0.5}\text{BiS}_2$ with high-entropy-alloy-type blocking layers. Applied Physics Express, 2018, 11, 053102.	1.1	53
2033	Adsorption Free Energy of Single Amino Acids at the Rutile (110)/Water Interface Studied by Well-Tempered Metadynamics. Journal of Physical Chemistry C, 2018, 122, 11355-11363.	1.5	21
2034	Evidence for a pressure-induced spin transition in olivine-type LiFePO_4 triphylite. Physical Review B, 2018, 97, .	1.1	6
2035	Spintronics Detection of Interfacial Magnetic Switching in a Paramagnetic Tris(8-hydroxyquinoline)iron(III) Thin Film. Materials and Energy, 2018, , 167-199.	2.5	2
2036	Magnetic Sponge with Neutral/Ionic Phase Transitions. Advanced Science, 2018, 5, 1700526.	5.6	25
2037	Pressure-induced strong ferroelectric polarization in tetra-phase perovskite CsPbBr_3 . Physical Chemistry Chemical Physics, 2018, 20, 14718-14724.	1.3	71
2038	A single-phased warm-white-emitting $\text{K}_3\text{Y}(\text{PO}_4)_2\text{Dy}^{3+}, \text{Sm}^{3+}$ phosphor with tuneable photoluminescence for near-UV-excited white LEDs. Dyes and Pigments, 2018, 157, 72-79.	2.0	49
2039	Substituting Cs for MA on the surface of MAPbI_3 perovskite: A first-principles study. Computational Materials Science, 2018, 150, 411-417.	1.4	18
2040	Strain engineering on electronic structure and carrier mobility in monolayer GeP_3 . Journal Physics D: Applied Physics, 2018, 51, 235302.	1.3	47
2041	Bayesian-Driven First-Principles Calculations for Accelerating Exploration of Fast Ion Conductors for Rechargeable Battery Application. Scientific Reports, 2018, 8, 5845.	1.6	77
2042	Surface structure-dependent pyrite oxidation in relatively dry and moist air: Implications for the reaction mechanism and sulfur evolution. Geochimica Et Cosmochimica Acta, 2018, 228, 259-274.	1.6	58
2043	A high-pressure X-ray diffraction study of the crystalline phases in calcium aluminate cement paste. Cement and Concrete Research, 2018, 108, 38-45.	4.6	24
2044	Novel Photocatalyst Based on Metastable ZrSnO_4 Solid for Hydrogen and Oxygen Evolution. Chemistry Letters, 2018, 47, 723-725.	0.7	4
2045	The role of boundary conditions in tuning the electronic properties of the $(0\bar{1}1)$ $\text{LaAlO}_3/\text{SrTiO}_3$ interface. Computational Materials Science, 2018, 149, 354-359.	1.4	5
2046	Synthesis, crystal structure and optical absorption of $\text{NaInS}_2\text{-Se}$. Journal of Alloys and Compounds, 2018, 750, 409-413.	2.8	8

#	ARTICLE	IF	CITATIONS
2047	Investigation of Transport Parameters of Graphene-Based Nanostructures. Russian Physics Journal, 2018, 60, 1938-1945.	0.2	3
2048	First principle investigation of the mechanical properties of natural layered nanocomposite: Clinocllore as a model system for heterodesmic structures. Composite Structures, 2018, 202, 551-558.	3.1	22
2049	Manganese pyrosilicates as novel positive electrode materials for Na-ion batteries. Sustainable Energy and Fuels, 2018, 2, 941-945.	2.5	3
2050	Intrinsic point defects in In_2S_3 studied by means of hybrid density-functional theory. Journal of Applied Physics, 2018, 123, .	1.1	22
2051	Selenium isotope effect in the layered bismuth chalcogenide superconductor $\text{LaO}_{0.6}\text{F}_{0.4}\text{Bi}(\text{S},\text{Se})_2$. Physical Review B, 2018, 97, .	1.1	32
2052	The vanadate garnet $\text{Ca}_2\text{NaCd}_2\text{V}_3\text{O}_{12}$: a single-crystal X-ray diffraction study. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 460-464.	0.2	5
2053	Electronic and vibrational properties of V_2C -based MXenes: From experiments to first-principles modeling. Physical Review B, 2018, 97, .	1.1	162
2054	Crown Ethers and Their Alkali Metal Ion Complexes as Assembler Groups in Uranyl ^{IV} Organic Coordination Polymers with <i>cis</i> -1,3-, <i>cis</i> -1,2-, and <i>trans</i> -1,2-Cyclohexanedicarboxylates. Crystal Growth and Design, 2018, 18, 3167-3177.	1.4	25
2055	A first-principle investigation of the Li diffusion mechanism in the super-ionic conductor lithium orthothioborate Li_3BS_3 structure. Materials Letters, 2018, 219, 186-189.	1.3	9
2056	Thermal Stability Enhanced Tetraethylenepentamine/Silica Adsorbents for High Performance CO ₂ Capture. Industrial & Engineering Chemistry Research, 2018, 57, 4632-4639.	1.8	46
2057	A first principle comparative study of the ionic diffusivity in LiAlO_2 and NaAlO_2 polymorphs for solid-state battery applications. Physical Chemistry Chemical Physics, 2018, 20, 9824-9832.	1.3	16
2058	Dependence of H ₂ and CO ₂ selectivity on Cu oxidation state during partial oxidation of methanol on Cu/ZnO. Applied Catalysis A: General, 2018, 556, 64-72.	2.2	34
2059	Metamagnetism with $T_N = 97$ K in a layered assembly of paddlewheel $[\text{Ru}_2]$ units and TCNQ: an empirical rule for interlayer distances determining the magnetic ground state. Materials Chemistry Frontiers, 2018, 2, 497-504.	3.2	16
2060	Point Defects and p -Type Doping in ScN from First Principles. Physical Review Applied, 2018, 9, .	1.5	33
2061	First principles investigation of the unipolar resistive switching mechanism in an interfacial phase change memory based on a $\text{GeTe/Sb}_2\text{Te}_3$ superlattice. Japanese Journal of Applied Physics, 2018, 57, 04FE08.	0.8	7
2062	Uranyl ^{IV} Organic Coordination Polymers with <i>trans</i> -1,2-, <i>trans</i> -1,4-, and <i>cis</i> -1,4-Cyclohexanedicarboxylates: Effects of Bulky PPh_4^+ and PPh_3Me^+ Counterions. Crystal Growth and Design, 2018, 18, 2609-2619.	1.4	22
2063	Uranyl Ion Complexes with Chiral Malic and Citramalic, and Prochiral Citric and Tricarballic Acids: Influence of Coligands and Additional Metal Cations. European Journal of Inorganic Chemistry, 2018, 1016-1027.	1.0	18
2064	Anisotropic vacancy-mediated phonon mode softening in Sm and Gd doped ceria. Physical Chemistry Chemical Physics, 2018, 20, 10048-10059.	1.3	10

#	ARTICLE	IF	CITATIONS
2065	Heterolytic dissociative adsorption state of dihydrogen favored by interfacial defects. Applied Surface Science, 2018, 433, 862-868.	3.1	9
2066	Segregation and mechanical properties of Si, Fe and Ti on the Al/Al ₂ X _{0.5} Zr (X = Cu, Zn, Ag) coherent interfaces: First-principles calculations. Computational Materials Science, 2018, 141, 325-340.	1.4	6
2067	The effect of the host lattice on the optical properties of Bi ³⁺ in Ca _{1-x} O:Bi and Ca _{1-x} (OH) ₂ :Bi phosphors. Applied Surface Science, 2018, 433, 155-159.	3.1	5
2068	The doping sites in Eu ²⁺ -doped AlBiPO ₄ phosphors and their consequence on the photoluminescence excitation spectra. Journal of Solid State Chemistry, 2018, 258, 124-130.	1.4	9
2069	Investigation on charge density, piezoelectric and ferroelectric properties of (1-x)Ba(Zr _{0.2} Ti _{0.8})O ₃ -x(Ba _{0.7} Ca _{0.3})TiO ₃ lead-free piezoceramics. Journal of Materials Science: Materials in Electronics, 2018, 29, 1198-1208.	1.1	8
2070	Possible causes for rippling in a multivacancy graphene system. International Journal of Quantum Chemistry, 2018, 118, e25529.	1.0	5
2071	Rare earth ions doped K ₂ Ta ₂ O ₆ photocatalysts with enhanced UV-vis light activity. Applied Catalysis B: Environmental, 2018, 224, 451-468.	10.8	46
2072	Half metallic ferromagnetism in gallium and zinc doped chromium phosphide: First principles calculations. Materials Chemistry and Physics, 2018, 203, 65-72.	2.0	10
2073	Second-order elastic constants of hexagonal hydroxylapatite (P ₆ ₃) from <i>ab initio</i> quantum mechanics: Comparison between DFT functionals and basis sets. International Journal of Quantum Chemistry, 2018, 118, e25500.	1.0	19
2074	Structural and photocatalytic examination of CoMoO ₄ nanopowders synthesized by GNP method. Materials Research Bulletin, 2018, 98, 111-120.	2.7	20
2075	Enhancement of the optical absorption of carbon group elements doped ZnS in the visible light range. Renewable Energy, 2018, 117, 22-27.	4.3	30
2076	Efficient technique for computational design of thermoelectric materials. Computer Physics Communications, 2018, 222, 152-157.	3.0	21
2077	Influence of different synthesis methods on structure, morphology and luminescent properties of BiOCl:Eu ³⁺ phosphors and ¹⁶ O analysis. Journal of Materials Science: Materials in Electronics, 2018, 29, 186-194.	1.1	5
2078	Structural and Thermal Validations of Y ₃ Ba ₅ Cu ₈ O ₁₈ Composites Synthesized via Citrate Sol-Gel Spontaneous Combustion Method. Journal of Superconductivity and Novel Magnetism, 2018, 31, 1279-1286.	0.8	7
2079	Grain-boundary-rich mesoporous NiTiO ₃ micro-prism as high tap-density, super rate and long life anode for sodium and lithium ion batteries. Energy Storage Materials, 2018, 13, 329-339.	9.5	40
2080	The effect of oxygen molecule adsorption on lead iodide perovskite surface by first-principles calculation. Applied Surface Science, 2018, 428, 140-147.	3.1	39
2081	Atomic and electronic basis for solutes strengthened (010) anti-phase boundary of L1 ₂ Co ₃ (Al, TM): A comprehensive first-principles study. Acta Materialia, 2018, 145, 30-40.	3.8	40
2082	Co ²⁺ -doped diopside: crystal structure and optical properties. Physics and Chemistry of Minerals, 2018, 45, 443-461.	0.3	6

#	ARTICLE	IF	CITATIONS
2083	First-Principles Study of Electronic Structure, Mechanical, and Thermoelectric Properties of Ternary Palladates CdPd ₃ O ₄ and TlPd ₃ O ₄ . <i>Journal of Electronic Materials</i> , 2018, 47, 1871-1880.	1.0	4
2084	Crystal Growth Conditions of Types I and II Na ⁺ Si Clathrates by Evaporation of Na from a Na ⁺ Si ⁴⁻ Sn Solution. <i>Crystal Growth and Design</i> , 2018, 18, 351-355.	1.4	9
2085	Influence of Mg ²⁺ , SO ₄ ²⁻ and Na ⁺ ions of sea water in crude oil recovery: DFT and ab initio molecular dynamics simulations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2018, 539, 53-58.	1.2	2
2086	Strengthening effects of alloying elements W and Re on Ni ₃ Al: A first-principles study. <i>Computational Materials Science</i> , 2018, 144, 23-31.	1.4	27
2087	Structural stability and magnetic-exchange coupling in Mn-doped monolayer/bilayer MoS ₂ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 553-561.	1.3	37
2088	Onion-like carbon as dopant/modification-free electrocatalyst for [VO] ₂ ⁺ /[VO ₂] ⁺ redox reaction: Performance-control mechanism. <i>Carbon</i> , 2018, 127, 31-40.	5.4	11
2089	Competing ferromagnetic and anti-ferromagnetic interactions in iron nitride ϵ -Fe ₂ N. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 449, 582-589.	1.0	4
2090	Optical absorption spectra and g factor of MgO: Mn ²⁺ explored by ab initio and semi empirical methods. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 113, 194-200.	1.9	8
2091	First row transition metal atoms embedded in multivacancies in a rippled graphene system. <i>Applied Surface Science</i> , 2018, 435, 102-107.	3.1	4
2092	A hybrid functional study of native point defects in Cu ₂ SnS ₃ : implications for reducing carrier recombination. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 256-261.	1.3	12
2093	Introduction and a Quick Look at MUESR, the Magnetic Structure and mUon Embedding Site Refinement Suite. , 2018, , .		7
2094	New high-pressure phases in MOOH (M = Al, Ga, In). <i>American Mineralogist</i> , 2018, 103, 1906-1917.	0.9	14
2095	First-principles calculations of orientation dependence of Si thermal oxidation based on Si emission model. <i>Japanese Journal of Applied Physics</i> , 2018, 57, 04FB06.	0.8	3
2096	Study of Local Mechanical Properties of Fe ₇₈ Al ₂₂ Alloy. <i>Key Engineering Materials</i> , 2018, 784, 27-32.	0.4	1
2097	TDDFT Investigation of the Hybrid Organic Inorganic Perovskite: CH ₃ NH ₃ PbC ₃ . , 2018, , .		0
2098	Magnetic properties of rare earth rhenium oxides Ln_3ReO_7 ($\text{Ln} = \text{Tj}, \text{Et}, \text{Q}, \text{Yb}$). <i>Journal of Solid State Chemistry</i> , 2018, 347, 1-10.	0.5	1
2099	The evolution of the M1 local structure during preparation of VMoNbTeO catalysts for ethane oxidative dehydrogenation to ethylene. <i>RSC Advances</i> , 2018, 8, 35903-35916.	1.7	25
2100	Experimental and computational phase boundary mapping of Co ₄ Sn ₆ Te ₆ . <i>Journal of Materials Chemistry A</i> , 2018, 6, 24175-24185.	5.2	26

#	ARTICLE	IF	CITATIONS
2101	New insight into the structure of PuGaO ₃ from <i>ab initio</i> particle-swarm optimization methodology. <i>Journal of Materials Chemistry A</i> , 2018, 6, 22798-22808.	5.2	16
2102	The competition between mechanical stability and charge carrier mobility in MA-based hybrid perovskites: insight from DFT. <i>Journal of Materials Chemistry C</i> , 2018, 6, 12252-12259.	2.7	42
2103	Phase transitions of Sm ₃ NbO ₇ , (Sm _{1-x} Ln _x) ₃ NbO ₇ (<i>Ln</i> = Nd, Tj), <i>Journal of Applied Physics</i> , 2018, 126, 743-749.	0.5	4
2104	A Facile Method Using a Flux to Improve Quantum Efficiency of Submicron Particle Sized Phosphors for Solid-State Lighting Applications. <i>Ceramics</i> , 2018, 1, 38-53.	1.0	3
2105	Probing molecule-like isolated octahedra via phase stabilization of zero-dimensional cesium lead halide nanocrystals. <i>Nature Communications</i> , 2018, 9, 4691.	5.8	56
2106	Distortion program for analysis of structural distortions affecting X-ray diffraction patterns. <i>AIP Advances</i> , 2018, 8, 101334.	0.6	3
2107	Theoretical Elucidation of Am(III)/Cm(III) Separation Mechanism with Diamide-type Ligands Using Relativistic Density Functional Theory Calculation. <i>Inorganic Chemistry</i> , 2018, 57, 14513-14523.	1.9	22
2108	Reversible superdense ordering of lithium between two graphene sheets. <i>Nature</i> , 2018, 564, 234-239.	13.7	178
2109	Effect of Nonspherical Encapsulated Guests on the Volumetric Behavior of Structure H Clathrate Hydrates. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27631-27639.	1.5	6
2110	Unravelling the effect of charge dynamics at the plasmonic metal/semiconductor interface for CO ₂ photoreduction. <i>Nature Communications</i> , 2018, 9, 4986.	5.8	168
2111	Crystal structure and ferroelectric polarization of tetragonal (Bi _{1/2} Na _{1/2})TiO ₃ ·12BaTiO ₃ . <i>Japanese Journal of Applied Physics</i> , 2018, 57, 11UD05.	0.8	5
2112	ZnO/ZnS (hetero)structures: <i>ab initio</i> investigations of polytypic behavior of mixed ZnO and ZnS compounds. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 628-642.	0.5	25
2113	Frustration wave order in iron(II) oxide spinels. <i>Communications Physics</i> , 2018, 1, .	2.0	6
2114	Ultrahigh-Magnetic-Field Magnetization of Multi-Kagome-Strip (MKS) Lattice Spin-Frustrated Magnet K ₂ Mn ₃ (OH) ₂ (VO ₄) ₂ . <i>Journal of the Physical Society of Japan</i> , 2018, 87, 124701.	0.7	2
2115	Design strategy for ferroelectric-based polar metals with dimensionality-tunable electronic states. <i>Science China: Physics, Mechanics and Astronomy</i> , 2018, 61, 1.	2.0	8
2116	Origin of the Low Magnetic Moment in Fe ₂ AlTi: An <i>Ab Initio</i> Study. <i>Materials</i> , 2018, 11, 1732.	1.3	19
2117	Role of oxygen and chlorine impurities in $Sr_{1-x}Ca_xFe_2O_{7-\delta}$: A first-principles study. <i>Physical Review B</i> , 2018, 98, .	1.1	7
2118	Reexploring the cation ordering and magnetic cation substitution effects on the elastic anisotropy of aluminum spinels. <i>Journal of Applied Physics</i> , 2018, 124, 175901.	1.1	7

#	ARTICLE	IF	CITATIONS
2119	Water Adsorption on the $\hat{1}^2$ -Dicalcium Silicate Surface from DFT Simulations. Minerals (Basel), Tj ETQq0 0 0 rgBT /Oyerlock 10 Tf 50 742	0.8	21
2120	Identifying quasi-2D and 1D electrides in yttrium and scandium chlorides via geometrical identification. Npj Computational Materials, 2018, 4, .	3.5	32
2121	Magnetocrystalline anisotropy of $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \langle \text{mml:mrow} \langle \text{mml:msub} \langle \text{mml:mi} \text{Fe} \langle \text{mml:mi} \langle \text{mml:mn} \rangle 5 \langle \text{mml:mn} \rangle \langle \text{mml:r} \text{and its alloys with Co and} \langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \langle \text{mml:mrow} \langle \text{mml:mn} \rangle 5 \langle \text{mml:mn} \rangle \langle \text{mml:mi} \text{d} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:r} \text{elements: A combined first-principles and experimental study. Physical Review B, 2018, 98, .}$	1.1	17
2122	Synthesis of Bismuth Ferrite BiFeO_3 by solution combustion method. Journal of Physics: Conference Series, 2018, 1143, 012025.	0.3	14
2123	Revealing the role of nitrogen on hydride nucleation and stability in pure niobium using first-principles calculations. Superconductor Science and Technology, 2018, 31, 115007.	1.8	19
2124	An Ab Initio Study of Thermodynamic and Mechanical Stability of Heusler-Based Fe_2AlCo Polymorphs. Materials, 2018, 11, 1543.	1.3	12
2125	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of $\text{Ca}_{10}\text{V}_6\text{O}_{25}$. Inorganic Chemistry, 2018, 57, 15489-15499.	1.9	18
2126	Hydrothermal reaction of NaBiO_3 with transition-metal (Co, Ni, Cu) salts. Journal of the Ceramic Society of Japan, 2018, 126, 1005-1012.	0.5	4
2127	Data-Driven Design of Ecofriendly Thermoelectric High-Entropy Sulfides. Inorganic Chemistry, 2018, 57, 13027-13033.	1.9	207
2128	Normal-state properties of the antiperovskite oxide Sr_3SnO revealed by ^{119}Sn -NMR. Physical Review B, 2018, 98, .	1.1	11
2129	Three Different Modes of Association between Metal Cations in Heterometallic $\text{Uranyl}^{\text{Co}}$ and $\text{Uranyl}^{\text{Mn}}$ Species. European Journal of Inorganic Chemistry, 2018, 2018, 4465-4471.	1.0	3
2130	Importance of Feature Selection in Machine Learning and Adaptive Design for Materials. Springer Series in Materials Science, 2018, , 59-79.	0.4	21
2131	Esfuerzo de corte en Interfaces $\text{Fe}/\text{Fe}_3\text{O}_4$. Revista Materia, 2018, 23, .	0.1	0
2132	Numerical investigation for lithium isotope effect in ionic superconductor. Fusion Engineering and Design, 2018, 136, 205-209.	1.0	8
2133	Crystal structure, photocatalytic and dielectric property of ATiM_2O_8 (A: Mg, Tj ETQq0 0 0 rgBT /Oyerlock 10	1.0	10
2134	Spherical neutron polarimetry under high pressure for a multiferroic delafossite ferrite. Nature Communications, 2018, 9, 4368.	5.8	7
2135	NanoCrystal: A Web-Based Crystallographic Tool for the Construction of Nanoparticles Based on Their Crystal Habit. Journal of Chemical Information and Modeling, 2018, 58, 2380-2386.	2.5	28
2136	The dynamics of Fe oxidation in riebeckite: A model for amphiboles. American Mineralogist, 2018, 103, 1103-1111.	0.9	32

#	ARTICLE	IF	CITATIONS
2137	Lattice expansion and local lattice distortion in Nb- and La-doped SrTiO_3 single crystals investigated by x-ray diffraction and first-principles calculations. <i>Physical Review B</i> , 2018, 98, .	1.1	23
2138	Effect of Synthetic Method and Annealing Temperature on the Structure of Hollandite-Type Oxides. <i>Inorganic Chemistry</i> , 2018, 57, 14353-14361.	1.9	5
2139	Density Functional Perturbation Theory to Predict Piezoelectric Properties. , 0, , .		2
2140	Superconductivity in $\text{La}_{1-x}\text{Ce}_x\text{OBiSSe}$: Carrier doping by mixed valence of Ce ions. <i>Europhysics Letters</i> , 2018, 122, 17004.	0.7	9
2141	$\text{Li}_3\text{Cr}(\text{MoO}_4)_3$: a NASICON-type high specific capacity cathode material for lithium ion batteries. <i>Journal of Materials Chemistry A</i> , 2018, 6, 19107-19112.	5.2	21
2142	Raman Spectrum of the Organic-Inorganic Halide Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ from First Principles and High-Resolution Low-Temperature Raman Measurements. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21703-21717.	1.5	87
2143	Comparative studies of wurtzite and zincblende indium nitride/yttria-stabilized zirconia interfacial and electronic properties by first-principles calculations. <i>Japanese Journal of Applied Physics</i> , 2018, 57, 100304.	0.8	0
2144	Pressures Tuning the Band Gap of Organic-Inorganic Trihalide Perovskites (MAPbBr_3): A First-Principles Study. <i>Journal of Electronic Materials</i> , 2018, 47, 7204-7211.	1.0	12
2145	The Use of Cluster Expansions To Predict the Structures and Properties of Surfaces and Nanostructured Materials. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2401-2413.	2.5	41
2146	Inflexible stoichiometry in bulk pyrite FeS_2 as viewed by <i>in situ</i> and high-resolution X-ray diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 436-444.	0.5	12
2147	Machine learning material properties from the periodic table using convolutional neural networks. <i>Chemical Science</i> , 2018, 9, 8426-8432.	3.7	75
2148	Two-Dimensional $\text{CsAg}_5\text{Te}_3\text{S}_3$ Semiconductors: Multi-anion Chalcogenides with Dynamic Disorder and Ultralow Thermal Conductivity. <i>Chemistry of Materials</i> , 2018, 30, 7245-7254.	3.2	15
2149	Promising $\text{Er}^{3+}/\text{Yb}^{3+}$ -Codoped GdBiW_2O_9 Phosphor for Temperature Sensing by Upconversion Luminescence. <i>ACS Omega</i> , 2018, 3, 11088-11096.	1.6	25
2150	$\text{Na}_{1-x}\text{Sn}_2\text{P}_2$ as a new member of van der Waals-type layered tin pnictide superconductors. <i>Scientific Reports</i> , 2018, 8, 12852.	1.6	22
2151	Influence of structural disorder on the magnetic properties and electronic structure of $\text{YCo}_2\text{Mn}_2\text{Ni}$. <i>Physical Review B</i> , 2018, 98, .		
2152	NASICON-type $\text{NaMo}_2(\text{PO}_4)_3$: Electrochemical activity of the Mo+4 polyanion compound in Na-cell. <i>Electrochimica Acta</i> , 2018, 289, 168-174.	2.6	15
2153	Electrical half-wave rectification at ferroelectric domain walls. <i>Nature Nanotechnology</i> , 2018, 13, 1028-1034.	15.6	77
2154	Thermal Conductivity due to Spins in the Frustrated Two-Leg Spin Ladder System BiCu_2PO_6 . <i>Journal of the Physical Society of Japan</i> , 2018, 87, 074702.	0.7	2

#	ARTICLE	IF	CITATIONS
2155	Density Functional Characterization of the f -Relevant Electronic Transitions of Lanthanide-Doped Lu_2O_3 Luminescence Materials. <i>ChemPhysChem</i> , 2018, 19, 2947-2953.	1.0	17
2156	Novel persistent and tribo-luminescence from bismuth ion pairs doped strontium gallate. <i>Journal of Materials Chemistry C</i> , 2018, 6, 10367-10375.	2.7	49
2157	Origin of gypsum growth habit difference as revealed by molecular conformations of surface-bound citrate and tartrate. <i>CrystEngComm</i> , 2018, 20, 3581-3589.	1.3	11
2158	Identification of a secondary phase Ga_2O_3 (ZnO) _m in Ga-doped ZnO thermoelectric materials by a (3+1)-dimensional superspace model. <i>Journal of Applied Crystallography</i> , 2018, 51, 924-927.	1.9	3
2159	Multisite formation in gadolinium doped SrF_2 nanoparticles. <i>Journal of Alloys and Compounds</i> , 2018, 762, 500-507.	2.8	4
2160	Appearance of Lithium-Ion Conduction in a LaLiCoO Band Insulator: Possible Route to Oxide Electrolyte. <i>ACS Applied Energy Materials</i> , 2018, 1, 2546-2554.	2.5	8
2161	Crystal structure, electronic structure, optical and scintillation properties of self-activated Cs_4YbI_6 . <i>Journal of Luminescence</i> , 2018, 201, 460-465.	1.5	12
2162	Static and Fluctuating Magnetic Moments in the Ferroelectric Metal LiOsO_3 . , 2018, , .		3
2163	Magnetic and ^{151}Eu Mössbauer spectroscopic studies on rare earth bismuth sulfides, EuLnBiS_4 ($\text{Ln} = \text{Tj, ET, Q, O, O, rg, BT, O, Ylock}$)	1.4	1
2164	Growth of trigonal gadolinium fluoride in a glass-ceramic for scintillation and optical applications. <i>Journal of the European Ceramic Society</i> , 2018, 38, 4739-4748.	2.8	10
2165	Counterion-Controlled Formation of an Octanuclear Uranyl Cage with $\text{cis-1,2-Cyclohexanedicarboxylate}$ Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 6283-6288.	1.9	28
2166	Crystalline phase detection in glass ceramics by EPR spectroscopy. <i>Low Temperature Physics</i> , 2018, 44, 341-345.	0.2	13
2167	Universal geometric frustration in pyrochlores. <i>Nature Communications</i> , 2018, 9, 2619.	5.8	64
2168	Magnetic properties of $\text{Ce}_{1.5}\text{M}^{TM}0.5\text{Ge}_4\text{O}_{12}$ ($\text{M} = \text{Mn, Co}$; $\text{M}^{TM} = \text{Ni, Cu}$). <i>Journal of Solid State Chemistry</i> , 2018, 265, 339-344.	1.4	2
2169	Atomic-scale study of stacking faults in Zr hydrides and implications on hydride formation. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 315003.	0.7	3
2170	Electronic and Optical Properties of Sodium Niobate: A Density Functional Theory Study. <i>Advances in Materials Science and Engineering</i> , 2018, 2018, 1-9.	1.0	17
2171	Synthesis of amine-functionalized ZIF-8 with 3-amino-1,2,4-triazole by postsynthetic modification for efficient CO_2 -selective adsorbents and beyond. <i>Journal of Materials Chemistry A</i> , 2018, 6, 18912-18919.	5.2	87
2172	Research Update: Ca doping effect on the Li-ion conductivity in NASICON-type solid electrolyte $\text{LiZr}_2(\text{PO}_4)_3$: A first-principles molecular dynamics study. <i>APL Materials</i> , 2018, 6, .	2.2	31

#	ARTICLE	IF	CITATIONS
2173	Layered ferrimagnets constructed from charge-transferred paddlewheel [Ru ₂] units and TCNQ derivatives: the importance of interlayer translational distance in determining magnetic ground state. Dalton Transactions, 2018, 47, 11760-11768.	1.6	18

2174 The structural, electronic, and optical properties of organic-inorganic mixed halide perovskites CH

#	ARTICLE	IF	CITATIONS
2191	Synthesis and Electrochemical Performance of C-Base-Centered Lepidocrocite-like Titanates for Na-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2018, 1, 3630-3635.	2.5	12
2192	Anisotropic growth of gas-liquid precipitated ceria mesocrystals to wires several micrometers in length. <i>RSC Advances</i> , 2018, 8, 24370-24375.	1.7	3
2193	Theoretical and Experimental Investigations into Novel Oxynitride Discovery in the GaN-TiO ₂ System at High Pressure. <i>Crystals</i> , 2018, 8, 15.	1.0	5
2194	Sub-solidus phase equilibria in the YO _{1.5} -TaO _{2.5} system. <i>Journal of the European Ceramic Society</i> , 2018, 38, 4786-4798.	2.8	17
2195	Observation of high magnetocrystalline anisotropy on Co doping in rare earth free Fe ₂ P magnetic material. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	0
2196	Crystal Structure, Thermal Behavior, and Photocatalytic Activity of NaBiO ₃ ·nH ₂ O. <i>Inorganic Chemistry</i> , 2018, 57, 8903-8908.	1.9	26
2197	Cobalt spin states investigation of Ruddlesden-Popper La _{2-x} Sr _x CoO ₄ , using X-ray diffraction and infrared spectroscopy. <i>Journal of Magnetism and Magnetic Materials</i> , 2018, 465, 768-774.	1.0	21
2198	Improved Prediction of Nanoalloy Structures by the Explicit Inclusion of Adsorbates in Cluster Expansions. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18040-18047.	1.5	19
2199	Predicted Binary Compounds of Tin and Sulfur. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17067-17072.	1.5	6
2200	Structural Diversity and Electronic Properties of 3d Transition Metal Tetraphosphides, TMP ₄ (TM = V, Cr, Mn, and Fe). <i>Inorganic Chemistry</i> , 2018, 57, 9385-9392.	1.9	21
2201	Free-energy analysis of physisorption on solid-liquid interface with the solution theory in the energy representation. <i>Journal of Chemical Physics</i> , 2018, 149, 014504.	1.2	6
2202	An investigation of the chemical durability of hydrous and anhydrous rare-earth phosphates. <i>Journal of Nuclear Materials</i> , 2018, 509, 631-643.	1.3	12
2203	The structure of P ₂ C (Ca _{0.2} Co _{0.8})CoSi ₂ O ₆ pyroxene and the P ₂ C phase transition in natural and synthetic Ca-Mg-Fe ²⁺ pyroxenes. <i>Mineralogical Magazine</i> , 2018, 82, 211-228.	0.6	5
2204	Theoretical exploration of the abnormal trend in lattice thermal conductivity for monosilicates RE ₂ SiO ₅ (RE = Dy, Ho, Er, Tm, Yb and Lu). <i>Journal of the European Ceramic Society</i> , 2018, 38, 3539-3546.	2.8	49
2205	Compression of Wannier functions into Gaussian-type orbitals. <i>Computer Physics Communications</i> , 2018, 230, 27-37.	3.0	3
2206	DFT insight into the effect of potassium on the adsorption, activation and dissociation of CO ₂ over Fe-based catalysts. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14694-14707.	1.3	40
2207	Microstructure of ZrB ₂ -ZrN directionally solidified eutectic composite by arc-melting. <i>Journal of Asian Ceramic Societies</i> , 2018, 6, 102-107.	1.0	5
2208	Effect of solutes on ideal shear resistance and electronic properties of magnesium: A first-principles study. <i>Acta Materialia</i> , 2018, 153, 327-335.	3.8	21

#	ARTICLE	IF	CITATIONS
2209	Computational chemical analysis of Eu(III) and Am(III) complexes with pnicogen-donor ligands using DFT calculations. Dalton Transactions, 2018, 47, 14924-14931.	1.6	9
2210	Tuning the electronic and chemisorption properties of hexagonal MgO nanotubes by doping "Theoretical study. Applied Surface Science, 2018, 457, 1158-1166.	3.1	3
2211	Steering reduction and decomposition of peroxide compounds by interface interactions between MgO thin film and transition-metal support. Applied Surface Science, 2018, 459, 812-821.	3.1	8
2212	Discovering minimum energy pathways via distortion symmetry groups. Physical Review B, 2018, 98, .	1.1	14
2213	A first-principle study of NaMPO4 (M = Mn, Fe, Co, Ni) possible novel structures as cathode materials for sodium-ion batteries: Structural and electrochemical characterisation. Materials Chemistry and Physics, 2018, 219, 212-221.	2.0	14
2214	Strong chromate-adsorbent based on pyrrolic nitrogen structure: An experimental and theoretical study on the adsorption mechanism. Water Research, 2018, 145, 287-296.	5.3	39
2215	Correlation between microstructure and cathodoluminescence properties of Mg(OH) ₂ (brucite) nanoparticles: effect of synthesis method. CrystEngComm, 2018, 20, 5632-5640.	1.3	6
2216	Carrier Lifetimes and Polaronic Mass Enhancement in the Hybrid Halide Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ Physical Review Letters, 2018, 121, 086402.	2.9	76
2217	Electronic and vibrational properties of PbI ₂ : From bulk to monolayer. Physical Review B, 2018, 98, .	1.1	49
2218	Enhanced electrochemical performance of Li-rich cathode materials through microstructural control. Physical Chemistry Chemical Physics, 2018, 20, 23112-23122.	1.3	46
2219	Oxidation behavior with quantum dots formation from amorphous GaAs thin films. Philosophical Magazine, 2018, 98, 2965-2981.	0.7	1
2220	An experimental and theoretical investigation of the structure of synthesized ZnO powder. Chemical Physics, 2018, 513, 273-279.	0.9	9
2221	Electronic structure and thermophysical properties of U ₃ Si ₂ : A systematic first principle study. Journal of Nuclear Materials, 2018, 510, 360-365.	1.3	15
2222	Expanding pentafluorouranates: hydrothermal synthesis and characterization of NaUF_5 and $\text{NaUF}_5 \cdot \text{H}_2\text{O}$. RSC Advances, 2018, 8, 28642-28648.	1.7	12
2223	Preparation of a double-layer YBa ₂ Cu ₃ O _{7-x} /CeO ₂ film on a Hastelloy C276 metal substrate with buffer layers of LaMnO ₃ /MgO/Gd ₂ Zr ₂ O ₇ by laser chemical vapor deposition. Thin Solid Films, 2018, 662, 33-40.	0.8	5
2224	Two-Dimensional versus Three-Dimensional Self-Assembly of a Series of 5-Alkoxyisophthalic Acids. Langmuir, 2018, 34, 10739-10747.	1.6	3
2225	Magnetic properties of praseodymium-containing double perovskites (Ba _{1-x} Sr _x) ₂ PrRuO ₆ . Journal of Solid State Chemistry, 2018, 267, 1-5.	1.4	0
2226	Superconductivity in Layered Oxychalcogenide La ₂ O ₂ Bi ₃ AgS ₆ . Journal of the Physical Society of Japan, 2018, 87, 083704.	0.7	17

#	ARTICLE	IF	CITATIONS
2227	Spin-orbit coupling driven crossover from a starfruitlike nodal semimetal to Dirac and Weyl semimetal state in CaAuAs. <i>Physical Review B</i> , 2018, 98, .	1.1	29
2228	Nuclear Magnetic Field in Solids Detected with Negative-Muon Spin Rotation and Relaxation. <i>Physical Review Letters</i> , 2018, 121, 087202.	2.9	22
2229	Curvature and vacancies in graphene quantum dots. <i>Applied Surface Science</i> , 2018, 462, 540-548.	3.1	16
2230	Theory of superconductivity in hole-doped monolayer MoS ₂ . <i>Physical Review B</i> , 2018, 98, .	1.1	10
2231	Electrochemical Modification of Negative Thermal Expansion Materials in the Ta _x Nb _{1-x} VO ₅ Series. <i>Inorganic Chemistry</i> , 2018, 57, 10633-10639.	1.9	6
2232	Effect of oxygen vacancies on intrinsic dielectric permittivity of strontium titanate ceramics. <i>Journal of the Ceramic Society of Japan</i> , 2018, 126, 263-268.	0.5	22
2233	A Microporous Covalent-Organic Framework with Abundant Accessible Carbonyl Groups for Lithium-Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9443-9446.	7.2	431
2234	Revealing the local lattice strains and strengthening mechanisms of Ti alloys. <i>Computational Materials Science</i> , 2018, 152, 169-177.	1.4	29
2235	Radiation-damaged zircon under high pressures. <i>Physics and Chemistry of Minerals</i> , 2018, 45, 981-993.	0.3	20
2236	Y ₂ O ₃ :Eu ³⁺ nano-luminophore obtained by low temperature thermolysis of trivalent rare earth 5-sulfisophthalate precursors. <i>Ceramics International</i> , 2018, 44, 15700-15705.	2.3	11
2237	A Microporous Covalent-Organic Framework with Abundant Accessible Carbonyl Groups for Lithium-Ion Batteries. <i>Angewandte Chemie</i> , 2018, 130, 9587-9590.	1.6	38
2238	Minimal effect of stacking number on intrinsic cleavage and shear behavior of Ti _n +1AlC _n and Ta _n +1AlC _n MAX phases. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	3
2239	Zero-dimensional Cs ₄ EuX ₆ (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. <i>Journal of Materials Chemistry C</i> , 2018, 6, 6647-6655.	2.7	66
2240	Coexistence of ferroelectric phases and electric field induced structural transformation in sodium potassium bismuth titanate ceramics. <i>Journal of Applied Physics</i> , 2018, 123, 234101.	1.1	0
2241	Pyrophosphates AMoP ₂ O ₇ (A = Li and Na): Synthesis, structure and electrochemical properties. <i>Materials Research Bulletin</i> , 2018, 106, 170-175.	2.7	6
2242	Copper interstitial recombination centers in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \langle \text{mml:mrow} \langle \text{mml:msub} \langle \text{mml:mi} \text{Cu} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \text{13} \langle \text{mml:mi} \rangle \langle \text{mml:mathvariant="normal"} \text{N} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$. <i>Physical Review B</i> , 2018, 97, .	1.3	18
2243	Influence of Cu and Na incorporation on the thermodynamic stability and electronic properties of In_2S_3 . <i>Journal of Materials Chemistry C</i> , 2018, 6, 7226-7231.	2.7	14
2244	Closed Uranyl-Dicarboxylate Oligomers: A Tetranuclear Metallacycle with Uranyl Bridgeheads and 1,3-Adamantanediacetate Linkers. <i>Inorganic Chemistry</i> , 2018, 57, 7932-7939.	1.9	21

#	ARTICLE	IF	CITATIONS
2245	Synthesis and Stability of Sr _x Ni _y O _z Chromium Getter for Solid Oxide Fuel Cells. Journal of the Electrochemical Society, 2018, 165, F635-F640.	1.3	10
2246	Synthesis, Crystal Structure, and Thermoelectric Properties of Layered Antimony Selenides REOSbSe ₂ (RE = La, Ce). Journal of the Physical Society of Japan, 2018, 87, 074703.	0.7	15
2247	Phase equilibria in the ZrO ₂ -YO _{1.5} -TaO _{2.5} system at 1250 Å°C. Journal of the European Ceramic Society, 2018, 38, 4523-4532.	2.8	25
2248	The critical role of hydrogen on the stability of oxy-hydroxyl defect clusters in uranium oxide. Journal of Materials Chemistry A, 2018, 6, 11362-11369.	5.2	17
2249	Polarization fluctuations in the perovskite-structured ferroelectric $\text{AgNb}_3\text{O}_{11}$. Physical Review B, 2018, 97, .	1.1	20
2250	Variation of crystal structure, magnetization, and dielectric properties of Nd and Ba co-doped BiFeO ₃ multiferroics. International Journal of Applied Ceramic Technology, 2019, 16, 119-129.	1.1	19
2251	Equation of state and second-order elastic constants of portlandite Ca(OH) ₂ and brucite Mg(OH) ₂ . Physics and Chemistry of Minerals, 2019, 46, 101-117.	0.3	16
2252	Screening Doping Strategies To Mitigate Electron Trapping at Anatase TiO ₂ Surfaces. Journal of Physical Chemistry C, 2019, 123, 22358-22367.	1.5	34
2253	Impact of Titanium Dioxide Surface Defects on the Interfacial Composition and Energetics of Evaporated Perovskite Active Layers. ACS Applied Materials & Interfaces, 2019, 11, 32500-32508.	4.0	33
2254	Development of SnSe thin films through selenization of sputtered Sn-metal films. Journal of Materials Science: Materials in Electronics, 2019, 30, 15980-15988.	1.1	16
2255	Two-Dimensional Hybrid Halide Perovskite as Electrode Materials for All-Solid-State Lithium Secondary Batteries Based on Sulfide Solid Electrolytes. ACS Applied Energy Materials, 2019, 2, 6569-6576.	2.5	17
2256	Structures of (4-Y-C ₆ H ₄ CH ₂ NH ₃) ₂ Pb ₄ {Y = H, F, Cl, Br, I}: Tuning of Hybrid Organic Inorganic Perovskite Structures from Ruddlesden-Popper to Dion-Jacobson Limits. Chemistry of Materials, 2019, 31, 6145-6153.	3.2	62
2257	Organic-inorganic all-pseudocapacitive asymmetric energy storage devices. Nano Energy, 2019, 65, 104022.	8.2	52
2258	Strain engineering on the electronic states of two-dimensional GaN/graphene heterostructure. RSC Advances, 2019, 9, 26024-26029.	1.7	19
2259	Electrodeposition of Silver Vanadate Films: A Tale of Two Polymorphs. ChemPhysChem, 2019, 20, 2635-2646.	1.0	10
2260	Analysis of individual molecular dynamics snapshots simulating wetting of surfaces using spheroidal geometric constructions. Journal of Chemical Physics, 2019, 151, .	1.2	4
2261	Tunable magnetic and half-metallic properties of the two-dimensional electron gas in LaAlO ₃ /SrTiO ₃ (111) heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 18170-18178.	1.3	4
2262	First-principles identification of the origin for higher activity of surface doped carbon nanohorn: Impact on hydrogen storage. International Journal of Hydrogen Energy, 2019, 44, 23196-23209.	3.8	10

#	ARTICLE	IF	CITATIONS
2263	Covalently Bonded Pillared Layered Bromoplumbate with High Thermal Stability: High Capacitance Gain after Photoinduced Electron Transfer. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 30713-30718.	4.0	22
2264	Confinement-Enhanced Rapid Interlayer Diffusion within Graphene-Supported Anisotropic ReSe_2 Electrodes. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 31147-31154.	4.0	13
2265	An ab initio molecular dynamics study on the threshold displacement energies in yttrium aluminum garnet. <i>Journal of Applied Physics</i> , 2019, 126, 055701.	1.1	4
2266	Enhanced superconductivity by Na doping in SnAs-based layered compound $\text{Na}_{1+x}\text{Sn}_{2x}\text{As}_2$. <i>Japanese Journal of Applied Physics</i> , 2019, 58, 083001.	0.8	11
2267	Phase transitions and lattice dynamics in perovskite-type hydride $\text{Li}_{1-x}\text{MgH}_3$. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 505402.	0.7	2
2268	Lithium-ion conductivity and crystal structure of garnet-type solid electrolyte $\text{Li}_7\text{La}_3\text{Zr}_2\text{F}_{23}$ using single-crystal. <i>Journal of the Ceramic Society of Japan</i> , 2019, 127, 521-526.		
2269	Adsorption properties of advanced functional materials against gaseous formaldehyde. <i>Environmental Research</i> , 2019, 178, 108672.	3.7	57
2270	Strain tuned electronic and magnetic anisotropy in SrTiO_3 (110) surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 2685-2691.	0.9	1
2271	DFT Study of the Adsorption and Dissociation of Water on Clean, Defective, and Oxygen-Covered U_3Si_2 {001}, {110}, and {111} Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19453-19467.	1.5	13
2272	Novel highly efficient and thermally stable $\text{Ca}_2\text{GdTaO}_6:\text{Eu}^{3+}$ red-emitting phosphors with high color purity for UV/blue-excited WLEDs. <i>Journal of Alloys and Compounds</i> , 2019, 804, 93-99.	2.8	73
2273	Experimental and theoretical study of microstructural characteristics and phase stability in equiatomic CrFeMoV alloy. <i>Materials Characterization</i> , 2019, 154, 449-457.	1.9	2
2274	Electronic Structure, Morphological Aspects, Optical and Electrochemical Properties of RuO_2 Nanocrystals. <i>Electronic Materials Letters</i> , 2019, 15, 645-653.	1.0	5
2275	Epitaxial Dimers and Auger-Assisted Detrapping in PbS Quantum Dot Solids. <i>Matter</i> , 2019, 1, 250-265.	5.0	56
2276	An electronic structure governed by the displacement of the indium site in InS_6 octahedra: LnInS_2 (Ln = La, Ce, and Pr). <i>Dalton Transactions</i> , 2019, 48, 12272-12278.	1.6	8
2277	Tuning the Bi^{3+} -photoemission color over the entire visible region by manipulating secondary cations modulation in the $\text{Sc}_x\text{P}_{1-x}\text{O}_4:\text{Bi}^{3+}$ (0 ≤ x ≤ 1) solid solution. <i>Journal of Materials Chemistry C</i> , 2019, 7, 9865-9877.	2.7	48
2278	Adsorption and mechanistic study for phosphate removal by rice husk-derived biochar functionalized with Mg/Al-calcined layered double hydroxides via co-pyrolysis. <i>Composites Part B: Engineering</i> , 2019, 176, 107209.	5.9	129
2279	High CO_2 -tolerance oxygen permeation dual-phase membranes $\text{Ce}_{0.9}\text{Pr}_{0.1}\text{O}_2-\text{Pr}_{0.6}\text{Sr}_{0.4}\text{Fe}_{0.8}\text{Al}_{0.2}\text{O}_3$. <i>Journal of Alloys and Compounds</i> , 2019, 806, 500-509.	2.8	22
2280	The importance of cation-cation repulsion in the zircon-reidite phase transition and radiation-damaged zircon. <i>Mineralogical Magazine</i> , 2019, 83, 561-567.	0.6	6

#	ARTICLE	IF	CITATIONS
2281	Synthesis, Crystal Structure, and Enthalpies of Formation of Churchite-type REPO ₄ ·2H ₂ O (RE = Gd to Lu) Materials. <i>Crystal Growth and Design</i> , 2019, 19, 4641-4649.	1.4	20
2282	Co-emergence of magnetic order and structural fluctuations in magnetite. <i>Nature Communications</i> , 2019, 10, 2857.	5.8	43
2283	Ab initio analysis of the optical spectra and EPR parameters of Ni ²⁺ ions in CaF ₂ and CdF ₂ crystals. <i>Journal of Luminescence</i> , 2019, 214, 116577.	1.5	6
2284	Making It Clear: Exploring Crystal Structures by Constructing and Comparing See-Through Models. <i>Journal of Chemical Education</i> , 2019, 96, 1630-1639.	1.1	10
2285	High-flux dual-phase percolation membrane for oxygen separation. <i>Journal of the European Ceramic Society</i> , 2019, 39, 4882-4890.	2.8	22
2286	Effects of Transition Metal Substituents on Interfacial and Electronic Structure of CH ₃ NH ₃ PbI ₃ /TiO ₂ Interface: A First-Principles Comparative Study. <i>Nanomaterials</i> , 2019, 9, 966.	1.9	13
2287	Theoretical prediction of piezoelectric property of new LiNbO ₃ -type compound AlTiO ₃ . <i>MRS Advances</i> , 2019, 4, 531-537.	0.5	0
2288	Effect of Indium doping on the superconductivity of layered oxychalcogenide La ₂ O ₂ Bi ₃ Ag _{1-x} In _x S ₆ . <i>Journal of Physics: Conference Series</i> , 2019, 1293, 012001.	0.3	0
2289	Critical behaviour and magnetocaloric properties of hexagonal MnCo _{0.7} Fe _{0.3} Ge. <i>Materials Research Express</i> , 2019, 6, 116563.	0.8	2
2290	Computationally generated maps of surface structures and catalytic activities for alloy phase diagrams. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 22044-22051.	3.3	14
2291	Magnetic and structural properties of Ni-substituted magnetoelectric Co ₄ Nb ₂ O ₉ . <i>Physical Review B</i> , 2019, 100, .	1.1	12
2292	Study on CePtIn ₄ grown in a platelet-like morphology. <i>Solid State Communications</i> , 2019, 302, 113717.	0.9	2
2293	Practical GW scheme for electronic structure of 3d-transition-metal monoxide anions: ScO ⁺ , TiO ⁺ , CuO ⁺ , and ZnO ⁺ . <i>Journal of Chemical Physics</i> , 2019, 151, 134305.	1.2	9
2294	Phosphorus-Doping-Induced Surface Vacancies of 3D Na ₂ Ti ₃ O ₇ Nanowire Arrays Enabling High-Rate and Long-Life Sodium Storage. <i>Chemistry - A European Journal</i> , 2019, 25, 14881-14889.	1.7	19
2295	Electronic Structure of In ₃ X ₄ Se ₄ Electron Transport Layer for Chalcogenide/p-Si Heterojunction Solar Cells. <i>ACS Omega</i> , 2019, 4, 17762-17772.	1.6	23
2296	Differential Surface Elemental Distribution Leads to Significantly Enhanced Stability of PtNi-Based ORR Catalysts. <i>Matter</i> , 2019, 1, 1567-1580.	5.0	82
2297	Versatile Nature of Oxygen Vacancies in Bismuth Vanadate Bulk and (001) Surface. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6672-6678.	2.1	32
2298	Unveiling ionic diffusion in MgNiMnO ₄ cathode material for Mg-ion batteries via combined computational and experimental studies. <i>Journal of Solid State Electrochemistry</i> , 2019, 23, 3209-3216.	1.2	10

#	ARTICLE	IF	CITATIONS
2299	Doping effect of Nb on ionic polarization of SrTiO ₃ . Journal of the Ceramic Society of Japan, 2019, 127, 357-361.	0.5	10
2300	Electronic specific heat coefficient and magnetic properties of $Y\text{Fe}_2\text{O}_7$ Laves phases: A combined experimental and first-principles study. Physical Review B, 2019, 100, .	1.1	2
2301	Confinement-Directed Adsorption of Noble Gases (Xe/Kr) in MFM-300(M)-Based Metal-Organic Framework Materials. Journal of Physical Chemistry C, 2019, 123, 27531-27541.	1.5	19
2303	Massless Dirac fermions in stable two-dimensional carbon-arsenic monolayer. Physical Review B, 2019, 100, .	1.1	10
2304	Effect of molybdenum on structural, optical and microwave dielectric properties of copper tungstate. Journal of Materials Science: Materials in Electronics, 2019, 30, 20758-20769.	1.1	4
2305	Quantum Interference and Substantial Property Tuning in Conjugated <i>Z</i> -Ortho-Regio-Resistive Organic (ZORRO) Junctions. Nano Letters, 2019, 19, 8956-8963.	4.5	10
2306	Mechanisms for hydrogen evolution on transition metal phosphide catalysts and a comparison to Pt(111). Physical Chemistry Chemical Physics, 2019, 21, 24489-24498.	1.3	31
2307	High density of genuine growth twins in electrodeposited aluminum. Science Advances, 2019, 5, eaax3894.	4.7	17
2308	Intrinsic Thermal Shock Behavior of Common Rutile Oxides. Physics, 2019, 1, 290-300.	0.5	6
2309	Electro-Thermal Analysis and Edge Termination Techniques of High Current $\text{In}^2\text{-Ga}_2\text{O}_3$ Schottky Rectifiers. , 2019, , .		0
2310	Mechanisms and Dynamics of Mineral Dissolution: A New Kinetic Monte Carlo Model. Advanced Theory and Simulations, 2019, 2, 1900114.	1.3	18
2311	High-Energy Photon Spectroscopy Using All Solution-Processed Heterojunctioned Surface-Modified Perovskite Single Crystals. ACS Applied Materials & Interfaces, 2019, 11, 33399-33408.	4.0	10
2312	Exploration of the high temperature phase evolution of electrochemically modified Sc ₂ (WO ₄) ₃ via potassium discharge. Inorganic Chemistry Frontiers, 2019, 6, 2718-2726.	3.0	2
2313	Internal and external pressure in cubic perovskites: electronic structure effects and systematic accuracy from first principles. Electronic Structure, 2019, 1, 035001.	1.0	6
2314	Real-Time Evolution of the Electron Clouds of Transition Metal Ions: Possible Electron-Pairing Medium in Unconventional High-Temperature Superconductors. Journal of Superconductivity and Novel Magnetism, 2019, 32, 2711-2715.	0.8	0
2315	Molecular Junctions Inspired by Nature: Electrical Conduction through Noncovalent Nanobelts. Journal of Physical Chemistry B, 2019, 123, 8096-8102.	1.2	9
2316	Activation of atomically precise silver clusters on carbon supports for styrene oxidation reactions. RSC Advances, 2019, 9, 28019-28027.	1.7	25
2317	FeTiO_2 : A spin Jahn-Teller transition enhanced by cation substitution. Physical Review B, 2019, 100, .	1.1	7

#	ARTICLE	IF	CITATIONS
2318	Evaluation of interfacial stability and strength of cermets based on work function. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20706-20719.	1.3	2
2319	Ensemble Effect in Bimetallic Electrocatalysts for CO ₂ Reduction. <i>Journal of the American Chemical Society</i> , 2019, 141, 16635-16642.	6.6	238
2320	Quantitative Structural Characterization of Catalytically Active TiO ₂ Nanoparticles. <i>ACS Applied Nano Materials</i> , 2019, 2, 6268-6276.	2.4	10
2321	Effect of $\hat{\pm}$ phase on evolution of oxygen-rich layer on titanium alloys. <i>Transactions of Nonferrous Metals Society of China</i> , 2019, 29, 534-545.	1.7	12
2322	Crystal structures and magnetic properties of dimorphic Li ₃ O ₅ O ₄ . <i>Solid State Sciences</i> , 2019, 97, 106009.	1.5	0
2323	Effect of hydrostatic pressure and the emergence of half metallic ferromagnetism in rhodium oxide - A DFT+U perspective. <i>Computational Condensed Matter</i> , 2019, 21, e00425.	0.9	0
2324	Hydrothermal synthesis of KTi ₂ (PO ₄) ₃ , $\hat{\pm}$ -Ti(HPO ₄) ₂ ·H ₂ O and $\hat{\beta}$ -Ti(PO ₄) ₂ (H ₂ PO ₄)·2H ₂ O from a lepidocrocite-type titanate. <i>Journal of Asian Ceramic Societies</i> , 2019, 7, 361-367.	1.0	3
2325	Pressure-induced superconductivity in the layered pnictogen diselenide NdO _{0.8} F _{0.2} Sb _{1-x} Bi _x Se ₂ (x=0.3 and 0.7). <i>Physical Review B</i> , 2019, 100, .	1.1	3
2326	Hydrothermal synthesis and crystal structure of a fluorite-type Pb _{0.35} Bi _{0.65} O _{1.59} compound with photocatalytic activity. <i>Materials Letters</i> , 2019, 257, 126688.	1.3	6
2327	Surface treated nickel phosphide nanosheet with oxygen as highly efficient bifunctional electrocatalysts for overall water splitting. <i>Applied Surface Science</i> , 2019, 496, 143741.	3.1	7
2328	Bulk superconductivity in a four-layer-type Bi-based compound La ₂ O ₂ Bi ₃ Ag _{0.6} Sn _{0.4} S _{5.7} Se _{0.3} . <i>Scientific Reports</i> , 2019, 9, 13346.	1.6	10
2329	Monitoring the Crystal Structure and the Electrochemical Properties of Na ₃ (VO) ₂ (PO ₄) ₂ F through Fe ³⁺ Substitution. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 38808-38818.	4.0	28
2330	Comparison of the crystal chemistry of tellurium (VI), molybdenum (VI), and tungsten (VI) in double perovskite oxides and related materials. <i>Progress in Solid State Chemistry</i> , 2019, 56, 100251.	3.9	17
2331	Synthesis of metal chloride films: Influence of growth conditions on crystallinity. <i>Thin Solid Films</i> , 2019, 689, 137520.	0.8	3
2332	Superconductivity in LaRh ₂ Ga ₂ with Noncentrosymmetric Structure. <i>Inorganic Chemistry</i> , 2019, 58, 12733-12738.	1.9	3
2333	Density Functional Theory (DFT)-Based Bonding Analysis Correlates Ligand Field Strength with ⁹⁹ Ru Mössbauer Parameters of Ruthenium Nitrosyl Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 14024-14033.	1.9	13
2334	High throughput identification of Li ion diffusion pathways in typical solid state electrolytes and electrode materials by BV-Ewald method. <i>Journal of Materials Chemistry A</i> , 2019, 7, 1300-1306.	5.2	12
2335	Interatomic chemical bonding and charge correlation of optical, magnetic and dielectric properties of La _{1-x} Sr _x FeO ₃ multiferroics synthesized by solid-state reaction method. <i>Journal of Materials Science: Materials in Electronics</i> , 2019, 30, 4409-4426.	1.1	8

#	ARTICLE	IF	CITATIONS
2336	Hard x-ray spectroscopy of the itinerant magnets $R_{1-x}Fe_x$ <small>xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi>Fe</mml:mi><mml:msub><mml:mi>Fe</mml:mi></mml:msub></mml:mrow></small></small>		

#	ARTICLE	IF	CITATIONS
2354	Non-thermal plasma needle as an effective tool in dimethoate removal from water. <i>Journal of Environmental Management</i> , 2019, 246, 63-70.	3.8	31
2355	Modeling and spectral simulation of formic acid dimer in Ar matrix using ONIOM calculations. <i>Computational and Theoretical Chemistry</i> , 2019, 1161, 18-25.	1.1	5
2356	New hybrid phosphite (CH ₃ OH)Cd(H ₂ PO ₃) ₂ : Synthesis, characterization and application of nanocomposite. <i>Journal of Molecular Liquids</i> , 2019, 289, 111142.	2.3	1
2357	Exchange bias effect, ferroelectric property, primary bonding and charge density analysis of La _{1-x} Ce _x FeO ₃ multiferroics. <i>Materials Research Bulletin</i> , 2019, 118, 110512.	2.7	8
2358	Segregation of point defects at the CuInSe ₂ (001)/GaAs(001) interface. <i>Solid State Communications</i> , 2019, 299, 113652.	0.9	1
2359	Novel Ca ₂ GdTaO ₆ :Mn ⁴⁺ ,M (M = Li ⁺ , Na ⁺ , K ⁺ , and Mg ²⁺) red phosphors for plant cultivation light-emitting diodes: Synthesis and luminescence properties. <i>Journal of Luminescence</i> , 2019, 214, 116525.	1.5	38
2360	Surface Structure of Co ₃ O ₄ (111) under Reactive Gas-Phase Environments. <i>ACS Catalysis</i> , 2019, 9, 6380-6392.	5.5	27
2361	Nuclear magnetic resonance and theoretical simulation study on Cs ion co-adsorbed with other alkali cations on illite. <i>Applied Surface Science</i> , 2019, 489, 766-775.	3.1	9
2362	Homolytic cleavage of water on magnesia film promoted by interfacial oxide-metal nanocomposite. <i>Applied Surface Science</i> , 2019, 487, 1222-1232.	3.1	5
2363	Electronic structure, chemical bonding, optical, elastic and dynamical properties of MeB ₂ compounds: Effect of transition metal Me = Sc, Ti and Zr. <i>Computational Condensed Matter</i> , 2019, 21, e00406.	0.9	12
2364	Synthesis and stability of tantalum hydride at high pressures. <i>Physical Review B</i> , 2019, 99, .	1.1	20
2365	Structure and disorder in ice VII on the approach to hydrogen-bond symmetrization. <i>Physical Review B</i> , 2019, 99, .	1.1	20
2366	Development of Y ₂ O ₃ : Ho ³⁺ /Yb ³⁺ Upconverting Nanophosphors for Enhancing Solar Cell Efficiency of Dye-Sensitized Solar Cells. <i>IEEE Journal of Photovoltaics</i> , 2019, 9, 1040-1045.	1.5	23
2367	DFT-Assisted Solid-State NMR Characterization of Defects in Li ₂ MnO ₃ . <i>Inorganic Chemistry</i> , 2019, 58, 8347-8356.	1.9	21
2368	A Theoretical Study on the Inclusion of Fe, Cu, and Zn in Illite Clays. <i>Journal of Nanomaterials</i> , 2019, 2019, 1-14.	1.5	1
2369	Hydrothermal Crystal Growth of Mixed Valence Cs ₂ SbBr ₆ . <i>Crystal Growth and Design</i> , 2019, 19, 4090-4094.	1.4	8
2370	Intercalation of transition metals in aluminene bi-layers: An ab initio study. <i>Journal of Chemical Physics</i> , 2019, 150, 194702.	1.2	3
2371	Polarized neutron diffraction on a diamagnetic bismuth single crystal. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 485, 286-290.	1.0	1

#	ARTICLE	IF	CITATIONS
2372	Co-doped Na ₂ FePO ₄ F fluorophosphates as a promising cathode material for rechargeable sodium-ion batteries. <i>Solid State Sciences</i> , 2019, 93, 62-69.	1.5	25
2373	Effect of interfacial defects on the electronic properties of graphene/g-GaN heterostructures. <i>RSC Advances</i> , 2019, 9, 13418-13423.	1.7	9
2374	Effect of mono-halogen-substitution on the electron transporting properties of perylene diimides: A density functional theory study. <i>Journal of Molecular Liquids</i> , 2019, 287, 110968.	2.3	4
2375	High-pressure behavior of liebenbergite: The most incompressible olivine-structured silicate. <i>American Mineralogist</i> , 2019, 104, 580-587.	0.9	4
2376	Developing and Piloting Culturally Relevant Chemistry Pedagogy: Computer-Based VSEPR and Unit Cell Lesson Plans from Collaborative Exchange in East Africa. <i>Journal of Chemical Education</i> , 2019, 96, 1273-1277.	1.1	5
2377	Uniaxial magnetocrystalline anisotropy of tetragonal Mn Ga ₁₀₀ (50% ⁻ x% ⁻ 75) alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 489, 165308.	1.0	8
2378	Selenium Edge as a Selective Anchoring Site for Lithium-Sulfur Batteries with MoSe ₂ /Graphene-Based Cathodes. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 19986-19993.	4.0	67
2379	Blue-light-pumped wide-band red emission in a new Ce ³⁺ -activated oxide phosphor, BaCa ₂ Y ₆ O ₁₂ :Ce ³⁺ : Melt synthesis and photoluminescence study based on crystallographic analyses. <i>Journal of Alloys and Compounds</i> , 2019, 797, 1181-1189.	2.8	23
2380	Unraveling the role of Ti in the stability of positive layered oxide electrodes for rechargeable Na-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 14169-14179.	5.2	55
2381	Ab initio study on structural and electronic properties of ReOFeAs (Re: La, Sm, Nd, Ce, Gd) under hydrostatic pressure. <i>Journal of Physics Communications</i> , 2019, 3, 015013.	0.5	1
2382	Crystal Structures and Phase-Transitions Analysis of the Double Perovskites Sr ₂ Co _{1-x} Ni _x TeO ₆ (x% = 0.25). <i>Journal of Materials</i> , 2019, 48, 4866-4876.	1.0	3
2383	Investigation of the (100) Surface of the Ce ₃ Pd ₂₀ Si ₆ Intermetallic Cage Compound. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12355-12366.	1.5	3
2384	First-principles investigation of the concentration effect on equilibrium fractionation of Ca isotopes in forsterite. <i>Acta Geochimica</i> , 2019, 38, 497-507.	0.7	8
2385	Templated vanadium tellurites: Identifying the effects of low density attractions on inorganic layer topology. <i>Journal of Solid State Chemistry</i> , 2019, 273, 158-165.	1.4	3
2386	Exploring the rate dependence of phase evolution in P2-type Na _{2/3} Mn _{0.8} Fe _{0.1} Ti _{0.1} O ₂ . <i>Journal of Materials Chemistry A</i> , 2019, 7, 12115-12125.	5.2	15
2387	Template free synthesis of CdSnO ₃ micro-cuboids for dye sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 380, 111824.	2.0	18
2388	Optical Properties and Photocatalytic Applications of Two-Dimensional Janus Group-III Monochalcogenides. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11388-11396.	1.5	132
2389	Stability in water and electrochemical properties of the Na ₃ V ₂ (PO ₄) ₂ F ₃ Na ₃ (VO) ₂ (PO ₄) ₂ F solid solution. <i>Energy Storage Materials</i> , 2019, 20, 324-334.	9.5	45

#	ARTICLE	IF	CITATIONS
2390	Electronic structure properties of CuZn ₂ InTe ₄ and AgZn ₂ InTe ₄ quaternary chalcogenides. Journal of Applied Physics, 2019, 125, 155101.	1.1	17
2391	Structural, electronic and optical studies of Pb-free halide double perovskite Cs ₂ BiAgBr ₆ ; an mBJLDA approach. AIP Conference Proceedings, 2019, , .	0.3	0
2392	Magnetization-polarization cross-control near room temperature in hexaferrite single crystals. Nature Communications, 2019, 10, 1247.	5.8	51
2393	Effect of stoichiometry on electrical response and polydispersivity related to hopping polarization in EuTiO ₃ . Journal of Applied Physics, 2019, 125, 114102.	1.1	2
2394	Wettability of Fully Hydroxylated and Alkylated (001) $\hat{\pm}$ -Quartz Surface in Carbon Dioxide Atmosphere. Journal of Physical Chemistry C, 2019, 123, 9027-9040.	1.5	69
2395	Rapid One-Pot Synthesis and Photoelectrochemical Properties of Copper Vanadates. ACS Applied Energy Materials, 2019, 2, 2837-2847.	2.5	34
2396	Structure, optical and varying magnetic properties of insulating MCr ₂ O ₄ (M= Co, Zn, Mg and Cd) nanospinels. Journal of Alloys and Compounds, 2019, 790, 853-862.	2.8	37
2397	Improving the electron transport performance by changing side chains in sulfur-containing azaacenes: a combined theoretical investigation on free molecules and an adsorption system. New Journal of Chemistry, 2019, 43, 5414-5422.	1.4	3
2398	First-principles study of the ferroelectric phase of AgNbO ₃ . , 2019, , 137-159.		0
2399	Static Dielectric Constant of $\langle i \rangle^2 \langle /i \rangle$ -Ga ₂ O ₃ Perpendicular to the Principal Planes (100), (010), and (001). ECS Journal of Solid State Science and Technology, 2019, 8, Q3083-Q3085.	0.9	58
2400	Electronic Properties of SbTa _{1-x} Nb _x O ₄ : Phase-Related Distortions. Journal of the Electrochemical Society, 2019, 166, H3195-H3201.	1.3	6
2401	Scalable Synthesis of Ultrathin Mn ₃ N ₂ Exhibiting Room-Temperature Antiferromagnetism. Advanced Functional Materials, 2019, 29, 1809001.	7.8	67
2402	Data-enabled structure-property mappings for lanthanide-activated inorganic scintillators. Journal of Materials Science, 2019, 54, 8361-8380.	1.7	9
2403	Impact of Hydrogen on the Intermediate Oxygen Clusters and Diffusion in Fluorite Structured UO _{2+x} . Inorganic Chemistry, 2019, 58, 3774-3779.	1.9	3
2404	Junction-configuration-dependent interfacial electronic states of a monolayer MoS ₂ /metal contact. Journal of Materials Chemistry C, 2019, 7, 3607-3616.	2.7	22
2405	Uncovering the influence of metallic and non-metallic impurities on the ideal shear strength and ductility of Ti: An ab-initio study. Journal of Alloys and Compounds, 2019, 788, 413-421.	2.8	14
2406	Enhanced energy storage properties in A-site substituted Na _{0.5} Bi _{0.5} TiO ₃ ceramics. Journal of Alloys and Compounds, 2019, 792, 95-107.	2.8	29
2407	Effect of different synthesis methods on the morphology, optical behavior, and superior photocatalytic performances of Ag ₃ PO ₄ sub-microcrystals using white-light-emitting diodes. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 377, 14-25.	2.0	29

#	ARTICLE	IF	CITATIONS
2408	Na ₃ V ₂ (PO ₄) ₃ @Carbon Nanofibers: High Mass Loading Electrode Approaching Practical Sodium Secondary Batteries Utilizing Ionic Liquid Electrolytes. ACS Applied Energy Materials, 2019, 2, 2818-2827.	2.5	34
2409	Electronic structure, carrier mobility and strain modulation of CH (SiH, GeH) nanoribbons. Journal of Physics Condensed Matter, 2019, 31, 165502.	0.7	11
2410	Atomic-scale design of friction and energy dissipation. Physical Review B, 2019, 99, .	1.1	23
2411	Structure and binding in halide perovskites: Analysis of static and dynamic effects from dispersion-corrected density functional theory. APL Materials, 2019, 7, .	2.2	31
2412	Novel defect-fluorite pyrochlore sodium niobate nanoparticles: solution-phase synthesis and radiation tolerance analysis. Nanoscale, 2019, 11, 5489-5498.	2.8	7
2413	Adsorption of volatile organic and iodine compounds over silver-exchanged mordenites: A comparative periodic DFT study for several silver loadings. Applied Surface Science, 2019, 485, 56-63.	3.1	48
2414	Stress-sign-tunable Poisson's ratio in monolayer blue phosphorus oxide. Journal of Physics Condensed Matter, 2019, 31, 295702.	0.7	12
2415	Application of the CLAYFF and the DREIDING Force Fields for Modeling of Alkylated Quartz Surfaces. Langmuir, 2019, 35, 5746-5752.	1.6	15
2416	Improvement of superconducting properties by high mixing entropy at blocking layers in BiS ₂ -based superconductor REO _{0.5} FO _{0.5} BiS ₂ . Solid State Communications, 2019, 295, 43-49.	0.9	34
2417	Color tunable and energy transfer mechanism of Dy ³⁺ and Eu ³⁺ rare earth ions activated NaCaBi ₂ (PO ₄) ₃ eulytite type phosphor for NUV excitable warm white light emitting diodes. Optik, 2019, 186, 221-230.	1.4	21
2418	First principles study on new half-metallic ferromagnetic ternary zinc-based sulfide and telluride (Zn ₃ VS ₄ and Zn ₃ VTe ₄). Materials Research Express, 2019, 6, 076107.	0.8	5
2419	Hydrothermal synthesis and crystal structure of new red phosphors, KNaMF ₇ :Mn ⁴⁺ (M: Nb, Ta). Materials Research Bulletin, 2019, 115, 170-175.	2.7	16
2420	Half-metallic ferromagnetism in Tc and Ag doped MgO: An ab-initio study. Computational Condensed Matter, 2019, 20, e00386.	0.9	5
2421	Thermal Simulations of High Current In ² -Ga ₂ O ₃ Schottky Rectifiers. ECS Journal of Solid State Science and Technology, 2019, 8, Q3195-Q3201.	0.9	31
2422	Neutron Scattering Studies on 4f ² -Electron Multipoles in Pr-based Systems. Journal of the Physical Society of Japan, 2019, 88, 081005.	0.7	1
2423	Size Fractionation of Graphene Oxide via Solvent-Mediated Consecutive Charge Manipulation and Investigation of the Size Effect as Hole Transporting Layer in Perovskite Solar Cells. ChemNanoMat, 2019, 5, 776-783.	1.5	7
2424	Building a Library of Simulated Atom Probe Data for Different Crystal Structures and Tip Orientations Using TAPSim. Microscopy and Microanalysis, 2019, 25, 320-330.	0.2	7
2425	Low-temperature Raman high magnetic field x-ray diffraction study of magnetodielectric coupling in polycrystalline GdFeO ₃ . Physical Review B, 2019, 99, .	1.1	14

#	ARTICLE	IF	CITATIONS
2426	Difference in magnetic and ferroelectric properties between rhombohedral and hexagonal polytypes of AgFeO : A single-crystal study. <i>Physical Review B</i> , 2019, 99, .	1.1	6
2427	Charge Transport and Thermoelectric Properties of Carbon Sulfide Nanobelts in Single-Molecule Sensors. <i>Chemistry of Materials</i> , 2019, 31, 6506-6518.	3.2	14
2428	Nonhexagonal Na Sublattice Reconstruction in the Super-Ionic Conductor $\text{Na}_2\text{Zn}_2\text{TeO}_6$: Insights from Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4654-4663.	1.5	9
2429	Cation Distributions and Anion Disorder in $\text{Ba}_3\text{NbMO}_{8.5}$ ($M = \text{Tj, ET, Q, r, g, BT, O, Y, Fe}$)	3.2	28
2430	Improvement of energy storage properties with the reduction of depolarization temperature in lead-free $\text{Na}_0.5\text{Bi}_0.5\text{TiO}_3\text{-xAgTaO}_3$ ceramics. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	19
2431	Tuning the electrocatalytic properties of a Cu electrode with organic additives containing amine group for CO_2 reduction. <i>Journal of Materials Chemistry A</i> , 2019, 7, 5453-5462.	5.2	28
2432	Reaction pathways for HCN on transition metal surfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5274-5284.	1.3	4
2433	Superconductivity in Uncollapsed Tetragonal LaFe_2As_2 . <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1018-1023.	2.1	17
2434	Electronic structure of CeCo_1Fe_3 studied by X-ray photoelectron spectroscopy and first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2019, 787, 744-750.	2.8	3
2435	Effect of Bi Substitution on Thermoelectric Properties of SbSe ₂ -based Layered Compounds $\text{NdO}_{0.8}\text{F}_{0.2}\text{Sb}_{1-x}\text{Bi}_x\text{Se}_2$. <i>Journal of the Physical Society of Japan</i> , 2019, 88, 024705.	0.7	5
2436	Coupled phonons and magnetic orderings in GaFeO_3 : Raman and magnetization studies. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	17
2437	On the nature of trapped states in an MoS_2 two-dimensional semiconductor with sulfur vacancies. <i>Molecular Physics</i> , 2019, 117, 2058-2068.	0.8	12
2438	Structure, morphology and magnetodielectric investigations of $\text{BaTi}_{1-x}\text{Fe}_x\text{O}_3$ ceramics. <i>Journal of Materials Science: Materials in Electronics</i> , 2019, 30, 5706-5717.	1.1	10
2439	Influence of repeating sequence on structural and thermal stability of crystalline domain of <i>bombyx mori</i> silk fibroin. <i>Materials Research Express</i> , 2019, 6, 125356.	0.8	3
2440	Flat Band and Hole-induced Ferromagnetism in a Novel Carbon Monolayer. <i>Scientific Reports</i> , 2019, 9, 20116.	1.6	19
2441	Hardening tungsten carbide by alloying elements with high work function. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 994-1002.	0.5	2
2442	Density Functional Theory-Assisted ^{31}P and ^{23}Na Magic-Angle Spinning Nuclear Magnetic Resonance Study of the $\text{Na}_3\text{V}_2(\text{PO}_4)_4\text{F}_3$ $\text{Na}_3\text{V}_2(\text{PO}_4)_4$ Solid Solution: Unraveling Its Local and Electronic Structures. <i>Chemistry of Materials</i> , 2019, 31, 9759-9768.	3.2	28
2443	Infrared nano-spectroscopy of ferroelastic domain walls in hybrid improper ferroelectric $\text{Ca}_3\text{Ti}_2\text{O}_7$. <i>Nature Communications</i> , 2019, 10, 5235.	5.8	18

#	ARTICLE	IF	CITATIONS
2444	Nontrivial topology in the layered Dirac nodal-line semimetal candidate SrZnSb with distorted Sb square nets. <i>Physical Review B</i> , 2019, 100, .	1.1	2
2445	Coupled structural distortions, domains, and control of phase competition in polar SmBaMnO_6 . <i>Physical Review B</i> , 2019, 100, .	1.1	8
2446	Predicted rebound effects of insulator-metal transition temperature in tungsten doped VO_2 via first-principles method. <i>Journal of Applied Physics</i> , 2019, 126, .	1.1	4
2447	Spin polarization in the phase diagram of a FeS system. <i>Scientific Reports</i> , 2019, 9, 19947.	1.6	3
2448	Superconductivity in High-Entropy-Alloy Telluride $\text{AgInSnPbBiTe}_{5-x}$. <i>Journal of the Physical Society of Japan</i> , 2019, 88, 124708.	0.7	35
2449	Copper Minerals at Vesuvius Volcano (Southern Italy): A Mineralogical Review. <i>Minerals (Basel)</i> , 2019, 9, 14.	0.8	14
2450	Synthesis and crystal structure of a new bismuth tin titanate with the pyrochlore-type structure. <i>Journal of the Ceramic Society of Japan</i> , 2019, 127, 952-957.	0.5	1
2451	Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations. <i>Heliyon</i> , 2019, 5, e02908.	1.4	6
2452	Electroluminescence of Cr^{3+} and pseudo-Stark effect in $\text{In}^{2-}\text{Ga}_2\text{O}_3$ Schottky barrier diodes. <i>Journal of Applied Physics</i> , 2019, 126, 213104.	1.1	7
2453	Optical Study of the Electronic Structure and Lattice Dynamics of $\text{NdBaMn}_2\text{O}_6$ Single Crystals. <i>Scientific Reports</i> , 2019, 9, 18164.	1.6	16
2454	Effect of Gd and Co content on electrochemical and electronic properties of $\text{La}_{1.5}\text{Mg}_{0.5}\text{Ni}_7$ alloys: A combined experimental and first-principles study. <i>Journal of Alloys and Compounds</i> , 2019, 773, 131-139.	2.8	11
2455	Crystal chemistry of K-rich nepheline in nephelinite from Hamada, Shimane Prefecture, Japan. <i>Mineralogical Magazine</i> , 2019, 83, 239-247.	0.6	7
2456	Hydrothermal crystallization of VO_4^{3-} stabilized $\text{t-Gd}(\text{P,V})\text{O}_4:\text{Eu}^{3+}$ nanocrystals for remarkably improved and color tailorable luminescence. <i>Chemical Engineering Journal</i> , 2019, 357, 84-93.	6.6	17
2457	Spectroscopic and ab initio studies of the pressure-induced Fe^{2+} high-spin-to-low-spin electronic transition in natural triphylite LiTiPO_4 . <i>Physics and Chemistry of Minerals</i> , 2019, 46, 245-258.	0.3	0
2458	Spectroscopic investigations of calcium fluoroapatites doped with Bi^{3+} . <i>Journal of Luminescence</i> , 2019, 205, 237-242.	1.5	6
2459	Structure-Directing Effects of Counterions in Uranyl Ion Complexes with Long-Chain Aliphatic $\text{C}_{12}\text{H}_{25}\text{NO}_2$ -Dicarboxylates: 1D to Polycatenated 3D Species. <i>Inorganic Chemistry</i> , 2019, 58, 567-580.	1.9	28
2460	Effect of Two-Dimensional Crystal Orbitals on Fermi Surfaces and Electron Transport in Three-Dimensional Perovskite Oxides. <i>Angewandte Chemie</i> , 2019, 131, 5557-5566.	1.6	8
2461	Effect of Two-Dimensional Crystal Orbitals on Fermi Surfaces and Electron Transport in Three-Dimensional Perovskite Oxides. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5503-5512.	7.2	17

#	ARTICLE	IF	CITATIONS
2462	Carbyne as a fiber in metal-matrix nanocomposites: A first principle study. Computational Materials Science, 2019, 159, 187-193.	1.4	7
2463	Structural Evolution and High-Voltage Structural Stability of $\text{Li}(\text{Ni}_x\text{Mn}_y\text{Co}_z)\text{O}_2$ Electrodes. Chemistry of Materials, 2019, 31, 376-386.	3.2	60
2464	High-Pressure Synthesis of $\text{Lu}_2\text{Ni}_6\text{O}_6$ with Ferrimagnetism and Large Coercivity. Inorganic Chemistry, 2019, 58, 397-404.	1.9	28
2465	Exploration of high-pressure structural transition and electronic properties of BaFe_2S_3 . Journal of Physics Condensed Matter, 2019, 31, 115401.	0.7	2
2466	Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its Application to GeO_2/Ge Interfaces. Journal of Physical Chemistry C, 2019, 123, 1208-1218.	1.5	11
2467	Monoclinic SrIrO_3 a Dirac semimetal produced by non-symmorphic symmetry and spin-orbit coupling. Journal of Physics Condensed Matter, 2019, 31, 074001.	0.7	5
2468	Analysis of migration maps and features of magnetic properties of $\text{LiNi}_0.9\text{Mn}_0.1\text{PO}_4$ ($\text{M} = \text{Co, Mn}$) single crystals. Journal of Alloys and Compounds, 2019, 781, 571-581.	2.8	9
2469	Germanium Fluoride Nanocages as Optically Transparent n-Type Materials and Their Endohedral Metallofullerene Derivatives. Journal of the American Chemical Society, 2019, 141, 1672-1684.	6.6	10
2470	X-ray scintillator $\text{Gd}_2\text{O}_3:\text{Tb}^{3+}$ materials obtained by a rapid and cost-effective microwave-assisted solid-state synthesis. Journal of Alloys and Compounds, 2019, 777, 638-645.	2.8	23
2471	Inducement of ferromagnetic-metallic phase and magnetoresistance behavior in charged ordered monovalent-doped $\text{Pr}_{0.75}\text{Na}_{0.25}\text{MnO}_3$ manganite by Ni substitution. Solid State Sciences, 2019, 87, 64-80.	1.5	18
2472	Generalized stacking fault energies of Cr_2C_6 carbide: A first-principles study. Computational Materials Science, 2019, 158, 20-25.	1.4	12
2473	Glycine self-assembled on graphene enhances the solar absorbance performance. Carbon, 2019, 143, 329-334.	5.4	21
2474	Structural refinement, morphology and photocatalytic properties of $\text{I}^{2-}(\text{Ag}_{2-x}\text{Zn}_x)\text{MoO}_4$ microcrystals synthesized by the sonochemical method. Journal of Materials Science: Materials in Electronics, 2019, 30, 1322-1344.	1.1	12
2475	Luminescence of Sb^{3+} in closed shell transition metal oxides. Journal of Luminescence, 2019, 208, 394-401.	1.5	12
2476	Effect of La doping on structural, magnetic, and optical properties of KBiFe_2O_5 . Journal of Materials Science: Materials in Electronics, 2019, 30, 4318-4325.	1.1	8
2477	Tunable thermal expansion of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate. Journal of Physics Condensed Matter, 2019, 31, 125101.	0.7	7
2478	Coupling of Acetaldehyde to Crotonaldehyde on $\text{CeO}_2(111)$: Bifunctional Mechanism and Role of Oxygen Vacancies. Journal of Physical Chemistry C, 2019, 123, 8273-8286.	1.5	23
2479	Blue-yellow multicolor phosphor, Eu^{2+} -activated $\text{Li}_3\text{NaSiO}_4$: Excellent thermal stability and quenching mechanism. Journal of Alloys and Compounds, 2019, 776, 1016-1024.	2.8	35

#	ARTICLE	IF	CITATIONS
2480	The mechanism of defect induced hydroxylation on pyrite surfaces and implications for hydroxyl radical generation in prebiotic chemistry. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 244, 163-172.	1.6	26
2481	Chiral Discrete and Polymeric Uranyl Ion Complexes with (1 <i>R</i> ,3 <i>S</i>)-(+)-Camphorate Ligands: Counterion-Dependent Formation of a Hexanuclear Cage. <i>Inorganic Chemistry</i> , 2019, 58, 870-880.	1.9	22
2482	Swift Combustion Synthesis of $\text{PbLi}_2\text{Ti}_6\text{O}_{14}$ Anode for Lithium-Ion Batteries: Diffusional and Electrochemical Investigation. <i>Journal of the Electrochemical Society</i> , 2019, 166, A5122-A5130.	1.3	6
2483	Investigation of half-metallic ferromagnetism in hafnium and tantalum doped NiO for spintronic applications: A DFT study. <i>Current Applied Physics</i> , 2019, 19, 357-362.	1.1	4
2484	Data-Driven Materials Exploration for Li-Ion Conductive Ceramics by Exhaustive and Informatics-Aided Computations. <i>Chemical Record</i> , 2019, 19, 771-778.	2.9	37
2485	First principles study of structural, electronic and optical properties of Cs-doped $\text{CH}_3\text{NH}_3\text{PbI}_3$ for photovoltaic applications. <i>Vacuum</i> , 2019, 160, 440-444.	1.6	18
2486	Electronic and optical properties of SnO_2 (110)/ MAPbI_3 (100) interface by first-principles calculations. <i>Materials Research Express</i> , 2019, 6, 026312.	0.8	3
2487	The adsorption of dodecylamine and oleic acid on kaolinite surfaces: Insights from DFT calculation and experimental investigation. <i>Applied Surface Science</i> , 2019, 470, 27-35.	3.1	38
2488	Molecular dynamics investigation of substrate wettability alteration and oil transport in a calcite nanopore. <i>Fuel</i> , 2019, 239, 1149-1161.	3.4	35
2489	Predicted semiconducting beryllium sulfides in 3D and 2D configurations: Insights from first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2019, 781, 371-377.	2.8	8
2490	Comparative study of free-volume nanostructurization in glassy and crystalline As_2S_3 re-examined with annihilating positrons. <i>Journal of Non-Crystalline Solids</i> , 2019, 503-504, 98-102.	1.5	5
2491	Effect of the pH pre-adjustment on the formation of $\text{In}_2\text{W}_3\text{O}_{12}$ and $\text{In}_6\text{WO}_{12}$ powders: Cluster coordination and optical band gap. <i>Boletin De La Sociedad Espanola De Ceramica Y Vidrio</i> , 2020, 59, 2-14.	0.9	0
2492	The size dependence of optical properties in colloidal $\text{Zn}_x\text{Cd}_{1-x}\text{S}:\text{Mn}$ quantum dots in gelatin. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 115, 113709.	1.3	2
2493	Comprehensive study on the electronic and optical properties of $\hat{\Gamma}_4^{\pm}\text{-U}_3\text{O}_8$. <i>Computational Materials Science</i> , 2020, 171, 109264.	1.4	9
2494	A DFT+U study to report magnetic phase transition, electronic properties and half metallic ferromagnetism in palladium oxide using Hubbard method. <i>Materials Chemistry and Physics</i> , 2020, 241, 122263.	2.0	7
2495	Crystal structure and magnetic properties of $\text{Sr}_2\text{Ni}_{1-x}\text{Mg}_x\text{MoO}_6$ ($x = 0, 0.25, 0.5, \text{ and } 0.75$) polycrystals. <i>Solid State Sciences</i> , 2020, 99, 106008.	1.5	11
2496	Structure and cation distribution in superparamagnetic NiCrFeO_4 nanoparticles using Mössbauer study. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 497, 166047.	1.0	13
2498	Multi-phase ELAStic Aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. <i>Computer Physics Communications</i> , 2020, 247, 106863.	3.0	9

#	ARTICLE	IF	CITATIONS
2499	Structural environment of chloride ion-conducting solids based on lanthanum oxychloride. <i>Journal of the American Ceramic Society</i> , 2020, 103, 297-303.	1.9	15
2500	(Cu, Ag)-DOPED ZnS WITH WIDE VISIBLE LIGHT RANGE ABSORPTION FOR WATER SPLITTING: A THEORETICAL AND EXPERIMENTAL STUDY. <i>Surface Review and Letters</i> , 2020, 27, 1950139.	0.5	1
2501	Exploring the electronic structure and thermal properties of UAl ₃ using density functional theory calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 136, 109179.	1.9	3
2502	Equilibrium inter-mineral titanium isotope fractionation: Implication for high-temperature titanium isotope geochemistry. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 269, 540-553.	1.6	42
2503	Effect of halogens in MgO to predict half-metallic ferromagnetism: By first principles calculations. <i>Solid State Sciences</i> , 2020, 99, 106048.	1.5	7
2504	Role of morphology, crystal orientation and stoichiometry in the electrical response of perovskite EuTiO ₃ ceramics. <i>Journal of the European Ceramic Society</i> , 2020, 40, 1250-1257.	2.8	4
2505	Silicene, Siloxene, or Silicane? Revealing the Structure and Optical Properties of Silicon Nanosheets Derived from Calcium Disilicide. <i>Chemistry of Materials</i> , 2020, 32, 795-804.	3.2	59
2506	Nitrogen induced half metallic ferromagnetism in oxides of calcium and cadmium: A DFT perspective. <i>Materials Chemistry and Physics</i> , 2020, 243, 122336.	2.0	2
2507	Manganese behavior in hydroxyapatite crystals revealed by X-ray difference Fourier maps. <i>Ceramics International</i> , 2020, 46, 10585-10597.	2.3	9
2508	New Dimorphs of Na ₅ V(PO ₄) ₂ F ₂ as an Ultrastable Cathode Material for Sodium-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2020, 3, 1181-1189.	2.5	16
2509	Influence of Synthesis Routes on the Crystallography, Morphology, and Electrochemistry of Li ₂ MnO ₃ . <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 5939-5950.	4.0	20
2510	Single-atom transition metals supported on black phosphorene for electrochemical nitrogen reduction. <i>Nanoscale</i> , 2020, 12, 4903-4908.	2.8	107
2511	Pyroelectric power generation from the waste heat of automotive exhaust gas. <i>Sustainable Energy and Fuels</i> , 2020, 4, 1143-1149.	2.5	16
2512	The Structural Stability of P2-Layered Na-Based Electrodes during Anionic Redox. <i>Joule</i> , 2020, 4, 420-434.	11.7	89
2513	The optical properties of Bi ³⁺ and Sb ³⁺ in YNbTiO ₆ analysed by means of DOS and semi-empirical calculations. <i>Journal of Materials Chemistry C</i> , 2020, 8, 2086-2093.	2.7	11
2514	Catalytic activation of peroxymonosulfate using CeVO ₄ for phenol degradation: An insight into the reaction pathway. <i>Applied Catalysis B: Environmental</i> , 2020, 266, 118601.	10.8	136
2515	A durable VO ₂ (M)/Zn battery with ultrahigh rate capability enabled by pseudocapacitive proton insertion. <i>Journal of Materials Chemistry A</i> , 2020, 8, 1731-1740.	5.2	90
2516	Towards a white-emitting phosphor Ca ₁₀ V ₆ O ₂₅ based material. <i>Journal of Luminescence</i> , 2020, 220, 116990.	1.5	5

#	ARTICLE	IF	CITATIONS
2517	High-pressure responses of alkali metal hydrogen carbonates, RbHCO ₃ and CsHCO ₃ : Findings of new phases and unique compressional behavior. <i>Journal of Solid State Chemistry</i> , 2020, 283, 121139.	1.4	4
2518	A Bond Charge Model Ansatz for Intrinsic Bond Energies: Application to C-C Bonds. <i>Journal of Physical Chemistry A</i> , 2020, 124, 176-184.	1.1	2
2519	Effect of Sodium Content on the Electrochemical Performance of Li-Substituted, Manganese-Based, Sodium-Ion Layered Oxide Cathodes. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 2191-2198.	4.0	18
2520	Two-Dimensional (001) LaAlO ₃ /SrTiO ₃ Heterostructures with Adjustable Band Gap and Magnetic Properties. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 3134-3139.	4.0	11
2521	Atomic Scale Understanding of the Epitaxy of Perovskite Oxides on Flexible Mica Substrate. <i>Advanced Materials Interfaces</i> , 2020, 7, 1901265.	1.9	21
2522	Na _{3+x} (Sb _{1-x} Sn _x)S ₄ solid electrolytes (0 ≤ x ≤ 0.1) as sodium ion conductors. <i>Solid State Ionics</i> , 2020, 344, 115133.	1.3	11
2523	Generation of molybdenum hydride species via addition of molecular hydrogen across metal-oxygen bond at monolayer oxide/metal composite interface. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 2975-2988.	3.8	10
2524	Exsolution of Metallic Ru Nanoparticles from Defective, Fluorite-Type Solid Solutions Sm ₂ Ru _x Ce _{2-2x} O ₇ To Impart Stability on Dry Reforming Catalysts. <i>ACS Catalysis</i> , 2020, 10, 1923-1937.	5.5	70
2525	Electron Confinement and Magnetism of (LaTiO ₃) ₁ (SrTiO ₃) ₅ Heterostructure: A Diffusion Quantum Monte Carlo Study. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 643-650.	2.3	4
2526	A Flexible Potassium-Ion Hybrid Capacitor with Superior Rate Performance and Long Cycling Life. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 2424-2431.	4.0	59
2527	Fundamental Insights into Photoelectrocatalytic Hydrogen Production with a Hole-Transport Bismuth Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2020, 142, 318-326.	6.6	60
2528	Temperature dependent X-ray diffraction and Raman spectroscopy studies of polycrystalline YCrO ₃ ceramics across the T C ~ 460 K. <i>Journal of Raman Spectroscopy</i> , 2020, 51, 537-545.	1.2	10
2529	Absorption spectra, ligand field parameters and g factors of Cr ³⁺ doped Al_2O_3 laser crystal: <i>ab initio</i> calculations. <i>Physica Scripta</i> , 2020, 95, 044005.	1.2	10
2530	stretchy="false">[</mml:mo><mml:mn>1</mml:mn><mml:mover accent="true"><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:mover></mml:math> tilt grain boundary in BCC Fe.	1.4	37
2531	Effect of Ni substitution at Mn-site on structural and electronic properties of monovalent-doped Pr _{0.75} Na _{0.25} MnO ₃ manganite: Experimental and first principles LDA+U studies. <i>Physica B: Condensed Matter</i> , 2020, 579, 411904.	1.3	1
2532	Thickness effect on the structural, electronic and energetic properties of the cubic KMgF ₃ (001) surfaces: A first-principles study. <i>Applied Surface Science</i> , 2020, 506, 144678.	3.1	4
2533	NaV ₆ O ₁₅ : A promising cathode material for insertion/extraction of Mg ²⁺ with excellent cycling performance. <i>Nano Research</i> , 2020, 13, 335-343.	5.8	28
2534	Non-covalently self-assembled organic molecules graphene aerogels to enhance supercapacitive performance. <i>Applied Surface Science</i> , 2020, 508, 145192.	3.1	24

#	ARTICLE	IF	CITATIONS
2553	Metallic Monolayer Ta ₂ CS ₂ : An Anode Candidate for Li ⁺ , Na ⁺ , K ⁺ , and Ca ²⁺ Ion Batteries. ACS Applied Energy Materials, 2020, 3, 10695-10701.	2.5	23
2554	Understanding the Correlation between Oxide Ion Mobility and Site Distributions in Ba ₃ NbWO _{8.5} . Inorganic Chemistry, 2020, 59, 14245-14250.	1.9	11
2555	Elucidation of the high-voltage phase in the layered sodium ion battery cathode material P ₃ Na _{0.5} Ni _{0.25} Mn _{0.75} O ₂ . Journal of Materials Chemistry A, 2020, 8, 21151-21162.	5.2	20
2556	High-speed epitaxial growth of Y ₃ Fe ₅ O ₁₂ thick film with high magnetization on (4 2 0) Y ₃ Al ₅ O ₁₂ substrate using metal-organic chemical vapor deposition. Materials Letters, 2020, 276, 128228.	1.3	3
2557	Novel electronic properties of monoclinic MP ₄ (M = Cr, Mo, W) compounds with or without topological nodal line. Scientific Reports, 2020, 10, 11502.	1.6	10
2558	A new process for the stabilization of vertically aligned Gd ₆ nanorods and their field emission properties. CrystEngComm, 2020, 22, 5473-5480.	1.3	6
2559	Fast and facile sonochemical synthesis of Mg- and Zn-doped PbS nanospheres: optical properties and photocatalytic activity. Journal of Materials Science: Materials in Electronics, 2020, 31, 14192-14202.	1.1	9
2560	Unexpected bowing band evolution in an all-inorganic CsSn _{1-x} Pb _x Br ₃ perovskite. RSC Advances, 2020, 10, 26407-26413.	1.7	4
2561	Lithium Iron Aluminum Nickelate, LiNi _x Fe _y Al _z O ₂ —New Sustainable Cathodes for Next-Generation Cobalt-Free Li-Ion Batteries. Advanced Materials, 2020, 32, e2002960.	11.1	77
2562	Theoretical analysis of doped graphene as cathode catalyst in Li-O ₂ and Na-O ₂ batteries—the impact of the computational scheme. Electrochimica Acta, 2020, 354, 136735.	2.6	11
2563	Diffusion of noble gases in subduction zone hydrous minerals. Geochimica Et Cosmochimica Acta, 2020, 291, 50-61.	1.6	4
2564	Effects of Mo on the mechanical behavior of β -strengthened Co-Ti-based alloys. Acta Materialia, 2020, 197, 69-80.	3.8	16
2565	Synchrotron radiation X-ray diffraction evidence for nature of chemical bonds in Bi ₄ Ti ₃ O ₁₂ ceramic powders and grain-orientation mechanism of their films formed by aerosol deposition method. Japanese Journal of Applied Physics, 2020, 59, SPPA04.	0.8	4
2566	Ferrites for Batteries. , 2020, , 147-172.		3
2567	Microscopic Hopping Mechanism of an Isolated PTCDA Molecule on a Reactive Ge(001) Surface. Journal of Physical Chemistry C, 2020, 124, 24704-24712.	1.5	2
2568	Investigation of the Inorganic Compounds NaMV ₂ (PO ₄) ₃ (M = Fe, Co, Ni) as Anode Materials for Sodium-Ion Batteries. ACS Omega, 2020, 5, 30799-30807.	1.6	4
2569	The effect of cation size on hydride-ion conduction in LnSrLiH ₂ O ₂ (Ln = La, Tj ETQq0 0 0 rgBT /Overlock 10 T	3.2	15
2570	Topological Analysis of Hydroxyquinoline Derivatives Interacting with Aluminum Cations or with an Al(111) Surface. Inorganic Chemistry, 2020, 59, 17916-17928.	1.9	2

#	ARTICLE	IF	CITATIONS
2571	Effective enhancement of thermoelectric and mechanical properties of germanium telluride <i>via</i> rhenium-doping. Journal of Materials Chemistry C, 2020, 8, 16940-16948.	2.7	38
2572	Alloy Design, Thermodynamics, and Electron Microscopy of Ternary Ti-Ag-Nb Alloy with Liquid Phase Separation. Materials, 2020, 13, 5268.	1.3	2
2573	Encapsulation of Highly Volatile Fragrances in Y Zeolites for Sustained Release: Experimental and Theoretical Studies. ACS Omega, 2020, 5, 31925-31935.	1.6	23
2574	Facile synthesis and thermoluminescence properties of nano bio-ceramic $\text{Ca}_2\text{P}_2\text{O}_7$:Dy phosphor irradiated with 75 Å MeV C_6^+ ion beam. Scientific Reports, 2020, 10, 21203.	1.6	10
2575	CO_2 Adsorption in Metal-Organic Framework Mg-MOF-74: Effects of Inter-Crystalline Space. Nanomaterials, 2020, 10, 2274.	1.9	18
2576	Methods for Lithium Ion NASICON Preparation: From Solid-State Synthesis to Highly Conductive Glass-Ceramics. Journal of Physical Chemistry C, 2020, 124, 26518-26539.	1.5	34
2577	Competing ferro- and antiferromagnetic exchange drives shape-selective Co_3O_4 nanomagnetism. Scientific Reports, 2020, 10, 20990.	1.6	9
2578	Unveiling Temperature-Induced Structural Domains and Movement of Oxygen Vacancies in SrTiO_3 with Graphene. ACS Applied Materials & Interfaces, 2020, 12, 52915-52921.	4.0	2
2579	Discovery and Single Crystal Growth of High Entropy Pyrochlores. Inorganic Chemistry, 2020, 59, 17251-17258.	1.9	11
2580	Comparative study on the resistance of different catalysts to electrochemical damage of fuel cells. International Journal of Hydrogen Energy, 2020, 45, 25249-25261.	3.8	2
2581	Evidence of room-temperature magnetodielectric effect in brownmillerite KBiFe_2O_5 through magnetic, complex dielectric, and impedance study. Journal of Materials Science: Materials in Electronics, 2020, 31, 15875-15884.	1.1	6
2582	Length scales of interfacial coupling between metal and insulator phases in oxides. Nature Materials, 2020, 19, 1182-1187.	13.3	42
2583	Control of energy dissipation in sliding low-dimensional materials. Physical Review B, 2020, 102, .	1.1	10
2584	Epitaxy from a Periodic O Monolayer: Growth of Single-Crystal Hexagonal YAlO_3 Perovskite. Nanomaterials, 2020, 10, 1515.	1.9	0
2585	Structural, electronic and magnetic properties of Sc^{3+} doped CoCr_2O_4 nanoparticles. New Journal of Chemistry, 2020, 44, 14246-14255.	1.4	31
2586	Computationally Guided Investigation of the Optical Spectra of Pure UO_3 . Inorganic Chemistry, 2020, 59, 11481-11492.	1.9	14
2587	Atomic-Scale Analysis of Biphasic Boundaries in the Lithium-Ion Battery Cathode Material LiFePO_4 . ACS Applied Energy Materials, 2020, 3, 8009-8016.	2.5	5
2588	Effects of the Bi^{3+} substitution on the structural, vibrational, and magnetic properties of bismuth layer-structured ferroelectrics. Applied Physics A: Materials Science and Processing, 2020, 126, 1.	1.1	8

#	ARTICLE	IF	CITATIONS
2589	Facet dependent catalytic activities of anatase TiO ₂ for CO ₂ adsorption and conversion. Applied Surface Science, 2020, 531, 147330.	3.1	16
2590	Synthesis and Dual-Mode Electrochromism of Anisotropic Monoclinic Nb ₁₂ O ₂₉ Colloidal Nanoplatelets. ACS Nano, 2020, 14, 10068-10082.	7.3	29
2591	Correlation between structure, dielectric and multiferroic properties of lead free Ni modified BaTiO ₃ solid solution. Ceramics International, 2020, 46, 27336-27351.	2.3	48
2592	A DFT study of the structural, elastic, electronic and magnetic properties of new quaternary compounds TiHfOsX(Al,Ga,In). Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126793.	0.9	11
2593	Li ₃ CaB ₂ O ₅ F: a unique sandwich-like structure with diverse and wide Li ion diffusion pathways. Dalton Transactions, 2020, 49, 12184-12188.	1.6	3
2594	Origin of the large ferroelectric polarization enhancement under high pressure for multiferroic DyMn_2O_7 studied by polarized and unpolarized neutron diffraction. Physical Review B, 2020, 102, .		
2595	Comparative Study on Sulfide and Oxide Electrolyte Interfaces with Cathodes in All-Solid-State Battery via First-Principles Calculations. ACS Applied Energy Materials, 2020, 3, 11061-11072.	2.5	19
2596	Effects of composition modulation on the type of band alignments for Pd ₂ Se ₃ /CsSnBr ₃ van der waals heterostructure: A transition from type I to type II. Journal of Power Sources, 2020, 478, 229078.	4.0	27
2597	Supercell-core software: A useful tool to generate an optimal supercell for vertically stacked nanomaterials. AIP Advances, 2020, 10, 105105.	0.6	4
2598	Undercoordinated Active Sites on 4H Gold Nanostructures for CO ₂ Reduction. Nano Letters, 2020, 20, 8074-8080.	4.5	46
2599	Monolayer Bi ₂ C ₃ : A promising sensor for environmentally toxic NCGs with high sensitivity and selectivity. Applied Surface Science, 2020, 534, 147609.	3.1	23
2600	High-pressure behaviour and phase stability of Ca ₂ B ₆ O ₆ (OH) ₁₀ ·2(H ₂ O) (meyerhofferite). Physics and Chemistry of Minerals, 2020, 47, 1.	0.3	6
2601	Carbon dioxide and water incorporation mechanisms in SrFeO _{3-δ} phases: a computational study. Physical Chemistry Chemical Physics, 2020, 22, 25146-25155.	1.3	4
2602	Hund's metal physics: From SrNiO ₂ to LaNiO ₂ . Physical Review B, 2020, 102, .	1.1	82
2603	Origin of High Nonradiative Recombination and Relevant Optoelectronic Properties of Ba ₂ Bi _{1-x} Nb _x O ₆ : Candidate for Photo(electro)catalysis and Photovoltaic Applications?. Advanced Optical Materials, 2020, 8, 2000901.	3.6	3
2604	Influence of the Processing Environment on the Surface Composition and Electronic Structure of Size-Quantized CdSe Quantum Dots. Journal of Physical Chemistry C, 2020, 124, 21305-21318.	1.5	9
2605	Luminescence in external dopant-free scandium-phosphorus vanadate solid solution: a spectroscopic and theoretical investigation. Materials Advances, 2020, 1, 2467-2482.	2.6	2
2606	One Structure, Two Elements—LuGe ₂ Superconductor vs Ordinary Metallic Conductor LuSn ₂ . A Case Study on How Site-Selective Germanium for Tin Atom Substitution Leads to Modulating of the Charge Distribution. Inorganic Chemistry, 2020, 59, 16853-16864.	1.9	7

#	ARTICLE	IF	CITATIONS
2607	A density functional theory study on the interface stability between CsPbBr ₃ and CuI. AIP Advances, 2020, 10, .	0.6	4
2608	Structural characterization and property modification for two-dimensional (001) SrTiO ₃ nanosheets. Applied Nanoscience (Switzerland), 2020, 10, 4273-4279.	1.6	8
2609	Oxidation and electrical properties of chromium-iron alloys in a corrosive molten electrolyte environment. Scientific Reports, 2020, 10, 14833.	1.6	9
2610	Strain-induced band modulation and excellent stability, transport and optical properties of penta-MP ₂ (M = Ni, Pd, and Pt) monolayers. Nanoscale Advances, 2020, 2, 4566-4580.	2.2	10
2611	Complexation and bonding studies on [Ru(NO)(H ₂ O) ₅] ³⁺ with nitrate ions by using density functional theory calculation. RSC Advances, 2020, 10, 24434-24443.	1.7	6
2612	How do students become experts? An in-depth study on the development of domain-specific awareness in a materials chemistry course. International Journal of Science Education, 2020, 42, 2032-2054.	1.0	4
2613	Isoelectronically substituted group-III based monolayers: An <i>ab initio</i> study. Physical Review B, 2020, 102, .	1.1	3
2614	Towards intermediate-band photovoltaic absorbers: theoretical insights on the incorporation of Ti and Nb in In ₂ S ₃ . Npj Computational Materials, 2020, 6, .	3.5	10
2615	Structural elucidation of microcrystalline MOFs from powder X-ray diffraction. Dalton Transactions, 2020, 49, 13897-13916.	1.6	33
2616	Pressure Induced Topological Quantum Phase Transition in Weyl Semimetal Td-MoTe ₂ . Journal of the Physical Society of Japan, 2020, 89, 094707.	0.7	4
2617	<i>In Situ</i> -Grown Cd ₂ S-Decorated ZnO Nanoparticles for Cr(VI) Sensing in Wastewater and a Theoretical Probe for Chromium-Induced Carcinogen Detection. ACS Applied Materials & Interfaces, 2020, 12, 43833-43843.	4.0	23
2618	Materials perspective on new lithium chlorides and bromides: insights into thermo-physical properties. Physical Chemistry Chemical Physics, 2020, 22, 22758-22767.	1.3	15
2619	Pressure-induced incommensurate antiferromagnetic order in a ferromagnetic B-site ordered double-perovskite Lu ₂ NiMnO ₆ . Physical Review B, 2020, 102, .	1.1	3
2620	Enhanced Hardness in High-Entropy Carbides through Atomic Randomness. Advanced Theory and Simulations, 2020, 3, 2000111.	1.3	68
2621	Predicting Feasible Modifications of Ce ₂ O ₃ Using a Combination of Global Optimization and Data Mining. Journal of Phase Equilibria and Diffusion, 2020, 41, 538-549.	0.5	10
2622	Thermodynamics and Mechanism of a Photocatalyzed Stereoselective [2 + 2] Cycloaddition on a CdSe Quantum Dot. Journal of the American Chemical Society, 2020, 142, 15488-15495.	6.6	13
2623	Dimensional crossover in Cr-doped $\text{Co}_{1-x}\text{Mn}_x$. Physical Review B, 2020, 102, .	1.3	5
2624	Suppressing the ferroelectric switching barrier in hybrid improper ferroelectrics. Npj Computational Materials, 2020, 6, .	3.5	20

#	ARTICLE	IF	CITATIONS
2625	Influence of Pr substitution on the physical properties of the $Ce_{1-x}Pr_xCoGe_3$ system: Combined experimental and first-principles study. <i>Physical Review B</i> , 2020, 102, .	1.1	5
2626	Stabilization of Competing Ferroelectric Phases of HfO_2 Epitaxial Strain. <i>Physical Review Letters</i> , 2020, 125, 257603.	2.9	46
2627	Structural Phase Diagram of $LaO_{1-x}F_xBiSSe$: Suppression of the Structural Phase Transition by Partial F Substitutions. <i>Condensed Matter</i> , 2020, 5, 81.	0.8	8
2628	Anion height dependence of critical current densities for $Fe_{1-x}Te_xSe_x$ bulk single crystals. <i>Journal of Physics: Conference Series</i> , 2020, 1590, 012013.	0.3	0
2629	Revisiting the antiferromagnet $NaNiO_2$ with muon spin rotation measurements and density functional theory calculations. <i>Physical Review B</i> , 2020, 102, .	1.1	4
2630	Performance controlled via surface oxygen-vacancy in Ti-based oxide catalyst during methyl oleate epoxidation. <i>Scientific Reports</i> , 2020, 10, 18952.	1.6	27
2631	Greigite (Fe_3S_4) is thermodynamically stable: Implications for its terrestrial and planetary occurrence. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 28645-28648.	3.3	12
2632	First-principle calculations of lithium adsorption and diffusion on titanium-based monolayers. <i>Chemical Physics</i> , 2020, 539, 110956.	0.9	3
2633	Bimetallic MOF-derived CNTs-grafted carbon nanocages as sulfur host for high-performance lithium-sulfur batteries. <i>Electrochimica Acta</i> , 2020, 349, 136378.	2.6	33
2634	Density functional theory and machine learning guided search for $RE_2Si_2O_7$ with targeted coefficient of thermal expansion. <i>Journal of the American Ceramic Society</i> , 2020, 103, 4489-4497.	1.9	16
2635	A new $Bi_0.7Fe_{1.3}O_{1.5}F_{1.7}$ phase: Crystal structure, magnetic properties, and cathode performance in fluoride-ion batteries. <i>APL Materials</i> , 2020, 8, .	2.2	11
2636	Preparation of MGF phosphor by O_2 postannealing and impact on luminescence properties and crystal lattice. <i>Journal of the American Ceramic Society</i> , 2020, 103, 5145-5156.	1.9	6
2637	Submicrostructure and Characteristics of the Short-Range Atomic Order in an Amorphous Ti-Ni-Ta-Zr-Based Surface Alloy Formed on a TiNi Substrate by the Electron-Beam Method. <i>Journal of Surface Investigation</i> , 2020, 14, 396-411.	0.1	1
2638	Hydrogen Trapping in bcc Iron. <i>Materials</i> , 2020, 13, 2288.	1.3	42
2639	Nanocrystals of Lead Chalcogenides: A Series of Kinetically Trapped Metastable Nanostructures. <i>Journal of the American Chemical Society</i> , 2020, 142, 10198-10211.	6.6	34
2640	Ab initio studies of the effect of the fluorination on deprotonation reaction of the benzene sulfonic acid. <i>Journal of Molecular Modeling</i> , 2020, 26, 127.	0.8	1
2641	Crystal Structure and Thermoelectric Transport Properties of As-Doped Layered Pnictogen Oxyselelenides $NdO_{0.8}F_{0.2}Sb_{1-x}As_xSe_2$. <i>Materials</i> , 2020, 13, 2164.	1.3	1
2642	First-principles insight into the entanglements between superionic diffusion and Li/Al antisite in Al-doped $Li_{1+x}Al_xGe_2(PO_4)_3$ (LAGP). <i>Science China Technological Sciences</i> , 2020, 63, 1787-1794.	2.0	7

#	ARTICLE	IF	CITATIONS
2643	Low temperature phonon studies and evidence of structureâ€“spin correlations in MnV ₂ O ₄ . Journal of Applied Physics, 2020, 127, .	1.1	5
2644	Superconductivity in Se-doped La ₂ O ₂ Bi ₂ Pb ₂ S _{6-x} Sex with a Bi ₂ Pb ₂ Ch ₄ -type thick conducting layer. Europhysics Letters, 2020, 129, 67001.	0.7	3
2645	Alkali metals inside bi-layer graphene and MoS ₂ : Insights from first-principles calculations. Nano Energy, 2020, 75, 104927.	8.2	30
2646	Effect of argon gas in oxygen catalytic recombination on a silica surface: A reactive molecular dynamics study. Acta Astronautica, 2020, 175, 531-539.	1.7	11
2647	A rational designed high-rate Cu _x Ti ₂ (PO ₄) ₃ @Cu/C core-composite-shell structure for aqueous lithium ion batteries. Journal of Power Sources, 2020, 468, 228248.	4.0	4
2648	High-speed epitaxial growth of M-type Strontium hexaferrite films on sapphire using metalâ€“organic chemical vapor deposition and their magnetic property. Materials Letters, 2020, 274, 128046.	1.3	9
2649	Plasma-Treated Ultrathin Ternary FePSe ₃ Nanosheets as a Bifunctional Electrocatalyst for Efficient Zincâ€“Air Batteries. ACS Applied Materials & Interfaces, 2020, 12, 29393-29403.	4.0	10
2650	Dopant arrangements in Y-doped BaZrO ₃ under processing conditions and their impact on proton conduction: a large-scale first-principles thermodynamics study. Journal of Materials Chemistry A, 2020, 8, 12674-12686.	5.2	25
2651	Bulk Superconductivity Induced by Se Substitution in Self-Doped BiCh ₂ -Based Compound CeOBiS ₂ . Journal of the Physical Society of Japan, 2020, 89, 064702.	0.7	3
2652	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
2653	Jahnâ€“Teller distortion-driven robust blue-light-emitting perovskite nanoplatelets. Applied Materials Today, 2020, 20, 100668.	2.3	11
2654	Mechanical and thermal properties of RETaO ₄ (RE = Yb, Lu, Sc) ceramics with monoclinic-prime phase. Journal of Materials Science and Technology, 2020, 52, 20-28.	5.6	40
2655	The chemical and physical properties of tetravalent lanthanides: Pr, Nd, Tb, and Dy. Dalton Transactions, 2020, 49, 15945-15987.	1.6	53
2656	Exploring high-energy and mechanically robust anode materials based on doped graphene for lithium-ion batteries: a first-principles study. RSC Advances, 2020, 10, 13662-13668.	1.7	10
2657	High-throughput screening platform for solid electrolytes combining hierarchical ion-transport prediction algorithms. Scientific Data, 2020, 7, 151.	2.4	90
2658	First-principles analysis of oxide-ion conduction mechanism in neodymium silicate. Solid State Ionics, 2020, 355, 115367.	1.3	2
2659	Computer Simulation of Spin Filtration Properties of Zigzag-Edged Octagraphene Nanoribbon Saturated with Hydrogen Atoms. Russian Physics Journal, 2020, 63, 303-310.	0.2	2
2660	Zinc-substituted Ag ₂ CrO ₄ : A material with enhanced photocatalytic and biological activity. Journal of Alloys and Compounds, 2020, 835, 155315.	2.8	16

#	ARTICLE	IF	CITATIONS
2661	Structure and glass transition of amorphous materials composed of titanium-oxo oligomers chemically modified with benzoylacetone. RSC Advances, 2020, 10, 15665-15669.	1.7	3

2662 High-performance Photodetector Based on $\ln_2\text{Se}_2\text{Cl}$

#	ARTICLE	IF	CITATIONS
2679	Magnetic properties of 6L-perovskites Ba ₃ Nd(Ru _{1-lr}) ₂ O ₉ showing hexagonal-monoclinic structural phase transition. Journal of Solid State Chemistry, 2020, 286, 121309.	1.4	0
2680	Heterobilayer CaS/CaSe: A promising sensor for environmental toxic NO ₂ gas with high selectivity and sensitivity. Applied Surface Science, 2020, 528, 146996.	3.1	30
2681	Two-dimensional O-phase group III monochalcogenides for photocatalytic water splitting. Journal of Physics Condensed Matter, 2020, 32, 065501.	0.7	6
2682	Synthesis, structure and characterization of three new Mg-containing phosphates with deep-UV cut-off edges. New Journal of Chemistry, 2020, 44, 6771-6777.	1.4	6
2683	On the spectroscopy of Bi ³⁺ in d10 post-transition metal oxides. Journal of Luminescence, 2020, 223, 117219.	1.5	30
2684	High-Pressure Synthesis and Superconducting Properties of NaCl-Type In ^{1-x} Pb _x Te (x = 0-0.8). Condensed Matter, 2020, 5, 14.	0.8	12
2685	Uptake of iodide by calcium aluminate phases (AFm phases). Applied Geochemistry, 2020, 116, 104559.	1.4	13
2686	Mott state of InMn_2Ir . <small>xmlns:mml="http://www.w3.org/1998/Math/MathML" <mml:msub><mml:mi>J</mml:mi><mml:mtext>eff</mml:mtext></mml:msub></small>	1.1	12
2687	Methylammonium tin iodide perovskite: structural, electronic and thermodynamic properties by a DFT study with different exchange correlation functionals. SN Applied Sciences, 2020, 2, 1.	1.5	14
2688	C-O bond activation using ultralow loading of noble metal catalysts on moderately reducible oxides. Nature Catalysis, 2020, 3, 446-453.	16.1	131
2689	Hydrothermal Synthesis and Crystal Structure of a Mixed-Valence Bismuthate, Na ₃ Bi ₃ O ₈ . Inorganic Chemistry, 2020, 59, 4950-4960.	1.9	13
2690	Femtosecond-laser-irradiation-induced structural organization and crystallinity of Bi ₂ WO ₆ . Scientific Reports, 2020, 10, 4613.	1.6	9
2691	GeC/GaN vdW Heterojunctions: A Promising Photocatalyst for Overall Water Splitting and Solar Energy Conversion. ACS Applied Materials & Interfaces, 2020, 12, 14289-14297.	4.0	62
2692	Balancing Dielectric Loss and Magnetic Loss in Fe ₂ /NiS/PVDF Composites toward Strong Microwave Reflection Loss. ACS Applied Materials & Interfaces, 2020, 12, 14416-14424.	4.0	136
2693	Electrical and mechanical properties and thermoelectric efficiency enhancement of monolayer and bilayer Si ₂ BN: A first-principle study. Chemical Physics, 2020, 538, 110908.	0.9	8
2694	A Novel Hyperbolic Two-Dimensional Carbon Material with an In-Plane Negative Poisson's Ratio Behavior and Low-Gap Semiconductor Characteristics. ACS Omega, 2020, 5, 15783-15790.	1.6	11
2695	Structural characterization, morphology, optical and colorimetric properties of NiWO ₄ crystals synthesized by the co-precipitation and polymeric precursor methods. Journal of Molecular Structure, 2020, 1221, 128774.	1.8	22
2696	Ultrathin Bi ₂ O ₂ S nanosheet near-infrared photodetectors. Nanoscale, 2020, 12, 16285-16291.	2.8	40

#	ARTICLE	IF	CITATIONS
2697	Electrochemical Evaluation of the Stability and Capacity of rGO-Wrapped Copper Antimony Chalcogenide Anode for Li-ion battery. ChemElectroChem, 2020, 7, 3291-3300.	1.7	9
2698	Magnetic Correlation Engineering in Spin-Sandwiched Layered Magnetic Frameworks. Chemistry - A European Journal, 2020, 26, 16755-16766.	1.7	4
2699	A Database of Ionic Transport Characteristics for Over 29 000 Inorganic Compounds. Advanced Functional Materials, 2020, 30, 2003087.	7.8	42
2700	Degradation of bisphenol A by peroxymonosulfate activated with oxygen vacancy modified nano-NiO-ZnO composite oxides: A typical surface-bound radical system. Chemical Engineering Journal, 2020, 400, 125915.	6.6	114
2701	Ab initio molecular dynamics simulation of threshold displacement energies and defect formation energies in Y4Zr3O12. Journal of Applied Physics, 2020, 127, .	1.1	10
2702	Phase-Pure Copper Vanadate (\pm -CuV ₂ O ₆): Solution Combustion Synthesis and Characterization. Chemistry of Materials, 2020, 32, 6247-6255.	3.2	27
2703	AA-Stacked Borophene-Graphene Bilayer with Covalent Bonding: Ab Initio Investigation of Structural, Electronic and Elastic properties. Journal of Physical Chemistry Letters, 2020, 11, 5668-5673.	2.1	34
2704	New layered perovskite family built from [CeTa ₂ O ₇] ⁿ⁺ layers: coloring mechanism from unique multi-transitions. Chemical Communications, 2020, 56, 8591-8594.	2.2	6
2705	Exploring the role of vacancy defects in the optical properties of LiMgPO ₄ . Physical Chemistry Chemical Physics, 2020, 22, 16244-16257.	1.3	41
2706	An in-situ electron microscopy study of dual ion-beam irradiated xenotime-type ErPO ₄ . Journal of Nuclear Materials, 2020, 539, 152265.	1.3	11
2707	Depression of direct exchange couplings in metallic glasses: A comparative study of critical and electronic behavior in Gd ₆ Co _{4.85} intermetallic compound and metallic glass. Intermetallics, 2020, 124, 106878.	1.8	2
2708	Construction of Single-Phase Nickel Disulfide Microflowers as High-Performance Electrodes for Hybrid Supercapacitors. Energy & Fuels, 2020, 34, 10178-10187.	2.5	27
2709	Low oxygen pressure synthesis of NdNiO ₃ - δ nanowires by electrospinning. Nano Express, 2020, 1, 010028.	1.2	5
2710	Novel method for the production of copper(II) formates, their thermal, spectral and magnetic properties. Journal of Alloys and Compounds, 2020, 845, 156208.	2.8	4
2711	Effect of Al doping on the structural and optical properties of CuO nanoparticles prepared by solution combustion method: Experiment and DFT investigation. Journal of Physics and Chemistry of Solids, 2020, 147, 109646.	1.9	39
2712	Computational discovery of two-dimensional HfO ₂ zoo based on evolutionary structure search. Physical Chemistry Chemical Physics, 2020, 22, 4481-4489.	1.3	5
2713	Off-stoichiometry effect on thermoelectric properties of the new p-type sulfides compounds Cu ₂ CoGeS ₄ . Journal of Alloys and Compounds, 2020, 826, 154240.	2.8	14
2714	Copper halide diselenium: predicted two-dimensional materials with ultrahigh anisotropic carrier mobilities. RSC Advances, 2020, 10, 8016-8026.	1.7	10

#	ARTICLE	IF	CITATIONS
2715	Stability of multiferroic phase and magnetization-polarization coupling in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{Y} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -type hexaferrite crystals. Physical Review B, 2020, 101, .	1.1	21
2716	First-principles study of the surface structure and stability of BC5. Materials Research Express, 2020, 7, 015617.	0.8	1
2717	Study on Ca Segregation toward an Epitaxial Interface between Bismuth Ferrite and Strontium Titanate. ACS Applied Materials & Interfaces, 2020, 12, 12264-12274.	4.0	5
2718	Crystal growth and Ce ³⁺ concentration optimization in Ti ₂ LaCl ₅ : An excellent scintillator for the radiation detection. Journal of Alloys and Compounds, 2020, 827, 154366.	2.8	23
2719	New Insights into the Role of Portlandite in the Cement System: Elastic Anisotropy, Thermal Stability, and Structural Compatibility with C-S-H. Crystal Growth and Design, 2020, 20, 2477-2488.	1.4	21
2720	Two-Dimensional 111-Type In -Based Halide Perovskite Cs ₃ In ₂ X ₉ (X=Cl,Br,I) with Optimal Band Gap for Photovoltaics and Defect-Insensitive Blue Emission. Physical Review Applied, 2020, 13, .	1.5	14
2721	Modulating Electronic Structures of Armchair GaN Nanoribbons by Chemical Functionalization under an Electric Field Effect. ACS Omega, 2020, 5, 1261-1269.	1.6	6
2723	Screening for Planar Carbon Allotropes Using Structure Space Sampling. Journal of Physical Chemistry C, 2020, 124, 6379-6384.	1.5	7
2724	Tunable Magnetic Exchange between Rare-Earth Metal 5d and Iron 3d States: A Case Study of the Multiple Magnetic Transitions in Gd ₆ FeBi ₂ and the Solid Solutions Dy ₆ Gd _x FeBi ₂ (1 ≤ x ≤ 5) with Curie Temperatures in the Range 120–350 K. Chemistry of Materials, 2020, 32, 3087-3096.	3.2	4
2725	Pressure-induced antiferromagnetic dome in the heavy-fermion $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Yb} \langle \text{mml:mi} \rangle \langle \text{mml:mfrac} \rangle \langle \text{mml:mn} \rangle 12 \langle \text{mml:mn} \rangle \langle \text{mml:mi} \rangle$ system. Physical Review B, 2020, 101, .		
2726	Layered $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{La} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \text{Cu} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$: A Promising Anisotropic Thermoelectric Material. Physical Review Applied, 2020, 13, .	1.5	80
2727	Particlelike Phonon Propagation Dominates Ultralow Lattice Thermal Conductivity in Crystalline $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{Ti} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mfrac} \rangle 3 \langle \text{mml:mfrac} \rangle \langle \text{mml:mi} \rangle$ Physical Review Letters, 2020, 124, 065901.	2.9	122
2728	Modeling of multi-scale transport phenomena in shale gas production – A critical review. Applied Energy, 2020, 262, 114575.	5.1	161
2729	The correlation between N deficiency and the mechanical properties of the Ti ₂ AlN _y MAX phase. Journal of the European Ceramic Society, 2020, 40, 2279-2286.	2.8	7
2730	Many-body renormalization of the electron effective mass of InSe. Physical Review B, 2020, 101, .	1.1	16
2731	Structural and electronic descriptors for atmospheric instability of Li-thiophosphate using density functional theory. Solid State Ionics, 2020, 346, 115225.	1.3	13
2732	Induced ferromagnetism and enhanced optical behaviour in indium-doped barium stannate system. Journal of Materials Science: Materials in Electronics, 2020, 31, 3375-3386.	1.1	6
2733	Structural and charge density distribution studies on Tin Oxide nanoparticles for Supercapacitor application. Journal of Energy Storage, 2020, 28, 101194.	3.9	30

#	ARTICLE	IF	CITATIONS
2734	Electronic Structure, Morphological Aspects, and Photocatalytic Discoloration of Three Organic Dyes with MgWO ₄ Powders Synthesized by the Complex Polymerization Method. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 2952-2970.	1.9	11
2735	Al/Ga-Doped Li ₇ La ₃ Zr ₂ O ₁₂ Garnets as Li-Ion Solid-State Battery Electrolytes: Atomistic Insights into Local Coordination Environments and Their Influence on ¹⁷ O, ²⁷ Al, and ⁷¹ Ga NMR Spectra. <i>Journal of the American Chemical Society</i> , 2020, 142, 3132-3148.	6.6	51
2736	Orbital Control and Coherent Charge Transport in Transition Metal Platinum(II)â€“Platinum(II) Lantern Complexes in Molecular Junctions. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3233-3241.	1.5	4
2737	Fabrication, structural and dielectric property of lead-free perovskite silver niobate ceramics. <i>Ceramics International</i> , 2020, 46, 12269-12274.	2.3	12
2738	Charge transport by global protonic conductivity and relaxational dynamics over hydrogen bonds in Fe ₂ +Fe ₃ +3.2(Mn ²⁺ ,Zn) _{0.8} (PO ₄) ₃ (OH) _{4.2} (HOH) _{0.8} . <i>Solid State Ionics</i> , 2020, 347, 115240.	1.3	4
2739	New Functionalities of Hydride Complexes with High Hydrogen Coordination. <i>Journal of the Physical Society of Japan</i> , 2020, 89, 051010.	0.7	3
2740	Deciphering the role of cationic substitution towards highly stable polyanionic cathodes. <i>Energy Storage Materials</i> , 2020, 29, 223-234.	9.5	10
2741	Investigation of the structural and electronic properties of InP _{1-x} Sb _x alloy for mid-infrared optoelectronic applications: A TB-mBJ DFT study. <i>Computational Condensed Matter</i> , 2020, 23, e00470.	0.9	3
2742	Salinity-dependent alterations of static and dynamic contact angles in oil/brine/calcite systems: A molecular dynamics simulation study. <i>Fuel</i> , 2020, 272, 117615.	3.4	26
2743	Superconductivity in La ₂ O ₂ M ₄ S ₆ -Type Bi-based Compounds: A Review on Element Substitution Effects. <i>Condensed Matter</i> , 2020, 5, 27.	0.8	5
2744	Quantum-Mechanical Assessment of the Energetics of Silver Decahedron Nanoparticles. <i>Nanomaterials</i> , 2020, 10, 767.	1.9	3
2745	Lattice-Parameter Dependence of Magnetic Structure in Orthorhombic YMnO ₃ . , 2020, , .		0
2746	Computational study of oxygen stability in vicinal m(10 ¹⁰)-GaN growth by MOVPE. <i>Applied Physics Express</i> , 2020, 13, 055507.	1.1	4
2747	Quantum-mechanical study of interaction between polycarbonate and M _{0.5} Al _{0.5} N(O ¹) surfaces (M ¹ =Ti), T _j E ₁ Q ₁ 1 0.784314 10.0		0
2748	Synthesis of RE ₁₂₃ high-T _c superconductors with a high-entropy-alloy-type RE site. <i>Physica C: Superconductivity and Its Applications</i> , 2020, 572, 1353623.	0.6	37
2749	Spin-torque switching of noncollinear antiferromagnetic antiperovskites. <i>Physical Review B</i> , 2020, 101, .	1.1	21
2750	Ultra-incompressibility and high energy density of ReN ₈ with infinite nitrogen chains. <i>Journal of Materials Science</i> , 2021, 56, 3814-3826.	1.7	9
2751	Sodiophilic Zn/SnO ₂ porous scaffold to stabilize sodium deposition for sodium metal batteries. <i>Chemical Engineering Journal</i> , 2021, 404, 126469.	6.6	35

#	ARTICLE	IF	CITATIONS
2752	A Pt/MnV ₂ O ₆ nanocomposite for the borohydride oxidation reaction. Journal of Energy Chemistry, 2021, 55, 428-436.	7.1	8
2753	Comparison of Arsenate Adsorption from Neutral pH Aqueous Solutions Using Two Different Iron-Trimesate Porous Solids: Kinetics, Equilibrium Isotherms, and Synchrotron X-Ray Absorption Experiments. Journal of Inorganic and Organometallic Polymers and Materials, 2021, 31, 1185-1194.	1.9	5
2754	Optical temperature sensor based on upconversion luminescence of Er ³⁺ doped GdTaO ₄ phosphors. Journal of the American Ceramic Society, 2021, 104, 361-368.	1.9	49
2755	Two-dimensional (Zr _{0.5} Hf _{0.5}) ₂ CO ₂ : A promising visible light water-splitting photocatalyst with efficiently carrier separation. Computational Materials Science, 2021, 186, 110013.	1.4	8
2756	Encapsulation ability of silicon carbide and boron nitride nanotubes for spilanthol molecule. Journal of Nanostructure in Chemistry, 2021, 11, 203-213.	5.3	9
2757	Molecular insights on the adsorption of some pharmaceutical residues from wastewater on kaolinite surfaces. Chemical Engineering Journal, 2021, 407, 127176.	6.6	46
2758	Sintering time dependent structural and magnetic phase transformations in Pr doped BiFeO ₃ multiferroics. Journal of Magnetism and Magnetic Materials, 2021, 519, 167412.	1.0	11
2759	Al ³⁺ -doping dependence on structural phase evolution in the LaCrO ₃ compound studied using atomistic simulation. Journal of Physics and Chemistry of Solids, 2021, 148, 109734.	1.9	2
2760	Viscosity of molten MgF ₂ -LiF-MgO system and structure investigation using classical molecular dynamics simulations. Journal of Non-Crystalline Solids, 2021, 552, 120377.	1.5	6
2761	2D Sb ₂ C ₃ monolayer: A promising material for the recyclable gas sensor for environmentally toxic nitrogen-containing gases (NCGs). Journal of Hazardous Materials, 2021, 405, 124168.	6.5	35
2762	Rheological properties and structure of molten FeO-TiO ₂ -B ₂ O ₃ ilmenite smelting slag. Journal of Non-Crystalline Solids, 2021, 552, 120308.	1.5	7
2763	NanoMaterialsCAD: Flexible Software for the Design of Nanostructures. Advanced Theory and Simulations, 2021, 4, 2000232.	1.3	2
2764	Hydrogen adsorption on calcium, potassium, and magnesium-decorations aluminene using density functional theory. International Journal of Hydrogen Energy, 2021, 46, 16676-16684.	3.8	7
2765	N, N-Dimethoxyimidazolium Derivatives as Ion Pair Constituents of Energetic Redox Couples: Model Studies by Thermal Analysis and Crystallography. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2021, 647, 365-376.	0.6	2
2766	Interfacial defect engineering on electronic states and electrical properties of MoS ₂ /metal contacts. Journal of Alloys and Compounds, 2021, 864, 158134.	2.8	6
2767	Piezo-response in two-dimensional ±-Tellurene films. Materials Today, 2021, 44, 40-47.	8.3	9
2768	Mechanistic insight of KBiQ ₂ (Q = S, Se) using panoramic synthesis towards synthesis-by-design. Chemical Science, 2021, 12, 1378-1391.	3.7	11
2769	Electronic, optical, and dielectric properties of OsP ₂ marcasite structure investigated by DFT calculations. Materials Science in Semiconductor Processing, 2021, 123, 105564.	1.9	1

#	ARTICLE	IF	CITATIONS
2770	Synthesis and characterization of the structural and magnetic properties of the $\text{Sm}_{3-x}\text{Gd}_x\text{Fe}_5\text{O}_{12}$ ($x=0.0, 0.2, 0.4, 0.6, 0.8, 1.0$). <i>Journal of Applied Physics</i> , 2021, 124, 124301. 2021, 859, 157883.	2.8	7
2771	Low-Index Stoichiometric Surfaces of $\text{CuBi}_2\text{W}_2\text{O}_8$. <i>Surface Science</i> , 2021, 705, 121762.	0.8	1
2772	Insight into enhanced thermoluminescence property of (Mg, Cu, Ag)-Doped LiF:A DFT study. <i>Journal of Luminescence</i> , 2021, 231, 117779.	1.5	8
2773	Effect of terbium and silver co-doping on the enhancement of photoluminescence in CaSO_4 phosphors. <i>Optical Materials</i> , 2021, 111, 110717.	1.7	3
2774	Improvement of bromide ion conduction in a lanthanum oxybromide-based solid by adjusting the electronegativity of the cation dopant. <i>Materials Letters</i> , 2021, 286, 129211.	1.3	3
2775	Prussian blue analogues as platform materials for understanding and developing oxygen evolution reaction electrocatalysts. <i>Journal of Catalysis</i> , 2021, 393, 390-398.	3.1	19
2776	Unveiling the interaction profile of cisplatin with gold-supported magnesia film. <i>Applied Surface Science</i> , 2021, 540, 148365.	3.1	8
2777	Ionic conduction mechanism in Ca-doped lanthanum oxychloride. <i>Dalton Transactions</i> , 2021, 50, 151-156.	1.6	7
2778	A highly efficient and informative method to identify ion transport networks in fast ion conductors. <i>Acta Materialia</i> , 2021, 203, 116490.	3.8	32
2779	Density functional modeling of $\text{Am}^{3+}/\text{Eu}^{3+}$ selectivity with diethylenetriaminepentaacetic acid and its bisamide chelates. <i>Journal of Nuclear Science and Technology</i> , 2021, 58, 515-526.	0.7	4
2780	Size-dependent phase transformation and its correlation with magnetic properties of multiferroic $0.8\text{BiFeO}_3 \cdot 0.2\text{CaTiO}_3$ nanoparticles. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 148, 109701.	1.9	1
2781	Nickel doped molybdenum oxide thin film counter electrodes as a low-cost replacement for platinum in dye sensitized solar cells. <i>Materials Today: Proceedings</i> , 2021, 39, 1856-1861.	0.9	10
2782	Hydrothermal synthesis of novel two-dimensional β -quartz nanoplates and their applications in energy-saving, high-efficiency, microalgal biorefineries. <i>Chemical Engineering Journal</i> , 2021, 413, 127467.	6.6	11
2783	High-rate capability of columbite CuNb_2O_6 anode materials for lithium-ion batteries. <i>Materials Letters</i> , 2021, 284, 128915.	1.3	30
2784	The Dionâ€“Jacobson perovskite CsSbCl_4 : a promising Pb-free solar-cell absorber with optimal bandgap ~ 1.4 eV, strong optical absorption $\sim 10^5 \text{ cm}^{-1}$, and large power-conversion efficiency above 20%. <i>Journal of Materials Chemistry A</i> , 2021, 9, 16436-16446.	5.2	13
2785	The interface interaction and photoelectric properties of the solar cell heterojunction CdS/CdMnTe : a first-principles study. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, .	0.2	3
2786	Characterization of N doped T-graphene and its application as an anode material for Na ion rechargeable batteries. <i>Sustainable Energy and Fuels</i> , 2021, 5, 4060-4068.	2.5	9
2787	Rietveld refinements, crystal structure and UV-Vis spectroscopy of MgO and $\text{Mg}(\text{OH})_2$ -based undoped and Sn^{4+} -doped MgTiO_3 ceramics. <i>Materials Today: Proceedings</i> , 2021, 45, 5249-5254.	0.9	1

#	ARTICLE	IF	CITATIONS
2788	Different structural evolutions of inorganic perovskite CsGe ₃ . CrystEngComm, 2021, 23, 4917-4922.	1.3	13
2789	Doping-Induced Combined Fano and Phonon Confinement Effect in La-Doped CeO ₂ : Raman Spectroscopy Analysis. Journal of Physical Chemistry C, 2021, 125, 2648-2658.	1.5	43
2790	Possible pairing mechanism switching driven by structural symmetry breaking in BiS ₂ -based layered superconductors. Scientific Reports, 2021, 11, 230.	1.6	9
2791	Tunable electronic and optical properties in buckling a non-lamellar B ₃ S monolayer. Physical Chemistry Chemical Physics, 2021, 23, 18669-18677.	1.3	4
2792	A proposed UML-based common model for information visualization systems. Multimedia Tools and Applications, 2021, 80, 12541-12579.	2.6	4
2793	Exploring the nature of the fergusonite-scheelite phase transition and ionic conductivity enhancement by Mo ⁶⁺ doping in LaNbO ₄ . Journal of Materials Chemistry A, 2021, 9, 4091-4102.	5.2	20
2794	Bond Valence Pathway Analyzer—An Automatic Rapid Screening Tool for Fast Ion Conductors within softBV. Chemistry of Materials, 2021, 33, 625-641.	3.2	112
2795	Characterization of the Ammonium Bending Vibrations in Two-Dimensional Hybrid Lead-Halide Perovskites from Raman Spectroscopy and First-Principles Calculations. Journal of Physical Chemistry C, 2021, 125, 223-236.	1.5	9
2796	Optimal water concentration for aqueous Li ⁺ intercalation in vanadyl phosphate. Chemical Science, 2021, 12, 4450-4454.	3.7	5
2797	A combined synchrotron diffraction and first-principles investigation on structural properties of Co(OH) ₂ under pressure up to 7 GPa. Europhysics Letters, 2021, 133, 16002.	0.7	1
2798	K _{1.5} VOPO ₄ F _{0.5} : a novel high-power and high-voltage cathode for rechargeable K-ion batteries. Journal of Materials Chemistry A, 2021, 9, 11802-11811.	5.2	8
2799	The First Principle Study of CuAgSe Subcells. Journal of Applied Mathematics and Physics, 2021, 09, 1549-1559.	0.2	0
2800	A DFT study of the adsorption energy and electronic interactions of the SO ₂ molecule on a CoP hydrotreating catalyst. RSC Advances, 2021, 11, 2947-2957.	1.7	49
2801	Novel copper fluoride analogs of cuprates. Physical Chemistry Chemical Physics, 2021, 23, 15989-15993.	1.3	5
2802	Latest directions in p-type transparent conductor design. Journal of Materials Chemistry C, 2021, 9, 11995-12009.	2.7	31
2803	Mapping surface morphology and phase evolution of iron sulfide nanoparticles. CrystEngComm, 2021, 23, 5645-5654.	1.3	4
2804	Nature of the magnetic stripes in fully oxygenated LaMnO_2 . Physical Review B, 2021, 103, .	5.2	31
2805	High-pressure structural phase transition and metallization in Ga ₂ S ₃ under non-hydrostatic and hydrostatic conditions up to 36.4 GPa. Journal of Materials Chemistry C, 2021, 9, 2912-2918.	2.7	20

#	ARTICLE	IF	CITATIONS
2806	Malate-aided selective crystallization and luminescence comparison of tetragonal and monoclinic LaVO_4 :Eu nanocrystals. Dalton Transactions, 2021, 50, 10147-10158.	1.6	8
2807	Development of a cyan blue-emitting $\text{Ba}_3\text{La}_2(\text{BO}_3)_4$: Ce^{3+} , Tb^{3+} phosphor for use in dental glazing materials: color tunable emission and energy transfer. RSC Advances, 2021, 11, 24949-24957.	1.7	4
2808	Non-invasively improving the Schottky barrier of MoS_2 /metal contacts by inserting a SiC layer. Physical Chemistry Chemical Physics, 2021, 23, 14796-14802.	1.3	6
2809	Towards bi-magnetic nanocomposites as permanent magnets through the optimization of the synthesis and magnetic properties of $\text{SrFe}_{12}\text{O}_{19}$ nanocrystallites. Journal Physics D: Applied Physics, 2021, 54, 124004.	1.3	17
2810	Phase Evolution of Trirutile $\text{Li}_{0.5}\text{FeF}_3$ for Lithium-Ion Batteries. Chemistry of Materials, 2021, 33, 868-880.	3.2	15
2811	Thermal equation of state of phase egg (AlSiO_3OH): implications for hydrous phases in the deep earth. Contributions To Mineralogy and Petrology, 2021, 176, 1.	1.2	2
2812	Identifying Highly Stable Structures of ABX_3 Compounds: Cases of CaTiO_3 and CsGeCl_3 Perovskites. , 2021, , .		0
2813	Strain Engineering for Tuning the Photocatalytic Activity of Metal-Organic Frameworks-Theoretical Study of the UiO-66 Case. Catalysts, 2021, 11, 264.	1.6	3
2814	Effect of Fluoroethylene Carbonate Additives on the Initial Formation of the Solid Electrolyte Interphase on an Oxygen-Functionalized Graphitic Anode in Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2021, 13, 8169-8180.	4.0	23
2815	Inelastic X-ray Scattering Study of the Cage-structured Compound $\text{PrRh}_2\text{Zn}_{20}$. Journal of the Physical Society of Japan, 2021, 90, 024602.	0.7	3
2816	Identification of embedded nanotwins at c-Si/a-Si:H interface limiting the performance of high-efficiency silicon heterojunction solar cells. Nature Energy, 2021, 6, 194-202.	19.8	52
2817	Investigation of Superconducting Properties and Possible Nematic Superconductivity in Self-Doped BiCh_2 -Based Superconductor $\text{CeOBiS}_{1.7}\text{Se}_{0.3}$. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2000546.	1.2	3
2818	Stabilization and electronic topological transition of hydrogen-rich metal $\text{Li}_5\text{MoH}_{11}$ under high pressures from first-principles predictions. Scientific Reports, 2021, 11, 4079.	1.6	12
2819	Synthetic Pathway Determines the Nonequilibrium Crystallography of Li- and Mn-Rich Layered Oxide Cathode Materials. ACS Applied Energy Materials, 2021, 4, 1924-1935.	2.5	15
2820	Density functional theory modeling of cation diffusion in tetragonal bulk ZrO_2 : Effects of humidity and hydrogen defect complexes on cation transport. Physical Review Research, 2021, 3, .	1.3	3
2821	4.7 V Operation of the $\text{Cr}^{4+}/\text{Cr}^{3+}$ Redox Couple in $\text{Na}_3\text{Cr}_2(\text{PO}_4)_4\text{F}_3$. Chemistry of Materials, 2021, 33, 1373-1379.	3.2	9
2822	Broken C_4 symmetry in the tetragonal state of uniaxial strained $\text{BaCo}_0.9\text{S}_{1.9}$. Physical Review Research, 2021, 3, .	1.3	1
2823	Tailoring c -Axis Orientation in Epitaxial Ruddlesden-Popper $\text{Pr}_{0.5}\text{Ca}_{1.5}\text{MnO}_4$ Films. Advanced Materials Interfaces, 2021, 8, 2002049.	1.9	2

#	ARTICLE	IF	CITATIONS
2824	Modeling the high-temperature phase coexistence region of mixed transition metal oxides from <i>ab initio</i> calculations. <i>Physical Review Research</i> , 2021, 3, .	1.3	4
2825	First-principles exploration of MgTi ₂ O ₅ and MgV ₂ O ₅ for CO ₂ capture and conversion. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26637.	1.0	3
2826	Crystallographic and optical bandgap study of LaFe _{1-x} Mg _x O ₃ (x=0.01 and 0.05) nanoparticle. <i>Journal of Physics: Conference Series</i> , 2021, 1816, 012065.	0.3	1
2827	Pressure-Induced Emergence of Visible Luminescence in Lead Free Halide Perovskite Cs ₃ Bi ₂ Br ₉ : Effect of Structural Distortion. <i>Journal of Physical Chemistry C</i> , 2021, 125, 3432-3440.	1.5	12
2828	Al ₂ O ₃ microparticles immobilized on glassy carbon electrode as catalytic sites for the electrochemical oxidation and high detectability of naproxen: Experimental and simulation insights. <i>Journal of Electroanalytical Chemistry</i> , 2021, 882, 114988.	1.9	13
2829	Structural phase transition in monolayer gold(I) telluride: From a room-temperature topological insulator to an auxetic semiconductor. <i>Physical Review B</i> , 2021, 103, .	1.1	10
2830	Magnetocaloric effect near room temperature and critical behaviour of Fe doped MnCo _{0.7} Fe _{0.3} Ge. <i>Solid State Communications</i> , 2021, 327, 114211.	0.9	4
2831	Rietveld refinement of the low temperature crystal structures of Cs ₂ XSi ₅ O ₁₂ (X = Cu, Cd and Zn). <i>European Journal of Chemistry</i> , 2021, 12, 60-63.	0.3	1
2832	Stacking fault energies of high-entropy nitrides from first-principles calculations. <i>Solid State Communications</i> , 2021, 327, 114210.	0.9	3
2833	First-Principles Calculations of SiBi Nanosheets as Sensors for Oxygen-Containing Gases. <i>ACS Applied Nano Materials</i> , 2021, 4, 2440-2451.	2.4	19
2834	Density Functional Theory Studies on Sulfur-Polyacrylonitrile as a Cathode Host Material for Lithium-Sulfur Batteries. <i>ACS Omega</i> , 2021, 6, 9700-9708.	1.6	11
2835	Photocatalytic activity of RBi ₂ O ₄ NO ₃ (R: Tb, Dy, Er, Gd, and Ho) for phenol degradation under visible light irradiation. <i>Journal of the Ceramic Society of Japan</i> , 2021, 129, 181-186.	0.5	2
2836	Low-Cost Computing of the Thermophysical Properties of Organic-Inorganic Halide Perovskites by Density Functional Theory Combined with the Three-Dimensional Reference Interaction Site Method. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6601-6610.	1.5	2
2837	Development of short and long-range magnetic order in the double perovskite based frustrated triangular lattice antiferromagnet Ba ₂ MnTeO ₆ . <i>Scientific Reports</i> , 2021, 11, 6959.	1.6	11
2838	Colossal Barocaloric Effect by Large Latent Heat Produced by First-Order Intersite Charge Transfer Transition. <i>Advanced Functional Materials</i> , 2021, 31, 2009476.	7.8	21
2839	Structural and magnetic properties of the quantum magnet BaCuTe ₂ O ₆ . <i>Physical Review B</i> , 2021, 103, .	1.1	3
2840	First-principles calculations for topological quantum materials. <i>Nature Reviews Physics</i> , 2021, 3, 283-297.	11.9	48
2841	Progress in state-of-the-art technologies of Ga ₂ O ₃ devices. <i>Journal Physics D: Applied Physics</i> , 2021, 54, 243001.	1.3	86

#	ARTICLE	IF	CITATIONS
2842	Anchoring Polysulfides and Accelerating Redox Reaction Enabled by Fe-Based Compounds in Lithium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2021, 31, 2100970.	7.8	94
2843	Experimental and computational investigation of Ti-Nb-Fe-Zr alloys with limited Fe contents for biomedical applications. <i>Journal of Materials Science</i> , 2021, 56, 11494-11510.	1.7	4
2844	Preferred orientations of garnet porphyroblasts reveal previously cryptic templating during nucleation. <i>Scientific Reports</i> , 2021, 11, 6869.	1.6	4
2845	Structure, Photoluminescence Emissions, and Photocatalytic Activity of Ag_2SeO_3 : A Joint Experimental and Theoretical Investigation. <i>Inorganic Chemistry</i> , 2021, 60, 5937-5954.	1.9	10
2846	Free energy of $(\text{CoMn}_{1-x})\text{Fe}_3\text{O}_4$ mixed phases from machine-learning-enhanced ab initio calculations. <i>Physical Review Materials</i> , 2021, 5, .	0.9	5
2847	Tuning the Magnetic Properties of Hard-Soft $\text{SrFe}_{12}\text{O}_{19}/\text{CoFe}_2\text{O}_4$ Nanostructures via Composition/Interphase Coupling. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5927-5936.	1.5	33
2848	Interfacial interactions and enhanced optoelectronic properties of GaN/perovskite heterostructures: insight from first-principles calculations. <i>Journal of Materials Science</i> , 2021, 56, 11352-11363.	1.7	7
2849	Synthesis and characterization of temperature stable low-loss $(1-x)\text{Mg}(\text{Ti}_{0.95}\text{Sn}_{0.05})\text{O}_3 \cdot x\text{BaTiO}_3$ ($0 \leq x \leq 0.1$) ceramics for microwave applications. <i>Journal of Materials Science</i> , 2021, 56, 10947-10964.	1.7	34
2850	<i>DATA</i> : a Python-based X-ray diffraction simulation code for arbitrary texture and arbitrary deformation. <i>Journal of Applied Crystallography</i> , 2021, 54, 686-696.	1.9	4
2851	HoHO: A Paramagnetic Air-Resistant Ionic Hydride with Ordered Anions. <i>Inorganic Chemistry</i> , 2021, 60, 3972-3979.	1.9	11
2852	Energetics for Twisted Bilayer of Circular Graphene Flake. <i>Journal of the Physical Society of Japan</i> , 2021, 90, 044602.	0.7	0
2853	An Ab Initio Perspective on the Key Vacancy Defects of KMgF_3 . <i>Journal of Physical Chemistry C</i> , 2021, 125, 8253-8267.	1.5	5
2854	Mechanistic Insights into Catalytic Reduction of N_2O by CO over Cu-Embedded Graphene: A Density Functional Theory Perspective. <i>ECS Journal of Solid State Science and Technology</i> , 2021, 10, 041003.	0.9	63
2855	Torsional moduli of transition metal dichalcogenide nanotubes from first principles. <i>Nanotechnology</i> , 2021, 32, 28LT02.	1.3	6
2856	Potassium-activated anionic copper and covalent Cu-Cu bonding in compressed K-Cu compounds. <i>Journal of Chemical Physics</i> , 2021, 154, 134708.	1.2	5
2857	In Situ Construction of Mo_2C Quantum Dots-Decorated CNT Networks as a Multifunctional Electrocatalyst for Advanced Lithium-Sulfur Batteries. <i>Small</i> , 2021, 17, e2100460.	5.2	81
2858	First-principles investigations on the electronic structures, polycrystalline elastic properties, ideal strengths and elastic anisotropy of U_3Si_2 . <i>European Physical Journal Plus</i> , 2021, 136, 1.	1.2	5
2859	Electrocatalytic activity of doped graphene: Quantum-mechanical theory view. <i>Carbon</i> , 2021, 175, 202-214.	5.4	7

#	ARTICLE	IF	CITATIONS
2860	Calculation of the band structure and density of localized states of materials of the quasi-binary system Zn ₃ As ₂ –Mn ₃ As ₂ . Solid State Communications, 2021, 328, 114237.	0.9	0
2861	An efficient method for large-scale preparation of high-purity $\hat{1}\pm$ -Si ₃ N ₄ nanowires and their electrochemical performance. Ceramics International, 2021, 47, 11304-11312.	2.3	3
2862	Material exploration via designing spatial arrangement of octahedral units: a case study of lead halide perovskites. Frontiers of Optoelectronics, 2021, 14, 252-259.	1.9	66
2863	Formation Mechanism of $\hat{1}^2$ -Li ₃ PS ₄ through Decomposition of Complexes. Inorganic Chemistry, 2021, 60, 6964-6970.	1.9	19
2864	Guanidinium tin halide perovskites: structural, electronic, and thermodynamic properties by quantum chemical study. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	5
2865	First-principles design of halide-reduced electrides: Magnetism and topological phases. Physical Review Materials, 2021, 5, .	0.9	5
2866	Atomic configurations for materials research: A case study of some simple binary compounds. AIP Advances, 2021, 11, .	0.6	4
2867	Predicting an ideal 2D carbon nanostructure with negative Poisson's ratio from first principles: implications for nanomechanical devices. Carbon Letters, 2021, 31, 1227-1235.	3.3	3
2868	Environmental-sulfur-controlled surface properties of pyrite: a first principles PBE+U study. Physics and Chemistry of Minerals, 2021, 48, 1.	0.3	6
2869	Birefringence and Dichroism in Quasi-1D Transition Metal Trichalcogenides: Direct Experimental Investigation. Small, 2021, 17, e2100457.	5.2	17
2870	Design and development of Ti–Zr–Hf–Nb–Ta–Mo high-entropy alloys for metallic biomaterials. Materials and Design, 2021, 202, 109548.	3.3	67
2871	Fabrication of a Facet-Oriented BiVO ₄ Photoanode by Particle Engineering for Promotion of Charge Separation Efficiency. ACS Applied Energy Materials, 2021, 4, 4259-4268.	2.5	16
2872	X-ray Nanoimaging of Crystal Defects in Single Grains of Solid-State Electrolyte Li ₃ AlLa ₃ Zr ₂ O ₁₂ . Nano Letters, 2021, 21, 4570-4576.	4.5	13
2873	Predicted half-metallicity and ferromagnetism in the Fe (III) doped BaZrO ₃ perovskite: A theoretical insight. AIP Advances, 2021, 11, 055104.	0.6	1
2874	Understanding Correlation Between CO ₂ Insertion Mechanism and Chain Length of Diamine in Metal-Organic Framework Adsorbents. ChemSusChem, 2021, 14, 2426-2433.	3.6	6
2875	Challenges in Rietveld Refinement and Structure Visualization in Ceramics. , 0, , .		8
2876	An approach based on random sampling and density functional theory to identify highly stable structures of ABX ₃ compounds. Computational Materials Science, 2021, 192, 110304.	1.4	2
2877	Electronic and crystal structures of LnFeAsO _{1-x} H _x (Ln = La, Sm) studied by x-ray absorption spectroscopy, x-ray emission spectroscopy, and x-ray diffraction (part I): Tj ETQq1 1 0.784314 r9BT /Overlock 10 TFS		

#	ARTICLE	IF	CITATIONS
2878	n-Type thermoelectric metal chalcogenide (Ag,Pb,Bi)(S,Se,Te) designed by multi-site-type high-entropy alloying. <i>Materials Research Letters</i> , 2021, 9, 366-372.	4.1	13
2879	Investigate the fast melting process of 2D SiC model by molecular dynamics. <i>Journal of Physics: Conference Series</i> , 2021, 1921, 012114.	0.3	0
2880	First-Principles DFT Study on Inverse Ruddlesden-Popper Tetragonal Compounds as Solid Electrolytes for All-Solid-State Li ⁺ -Ion Batteries. <i>Chemistry of Materials</i> , 2021, 33, 5859-5871.	3.2	13
2881	Effects of oxygen vacancy on the electrochemical properties of \hat{V}^3 -V ₂ O ₅ as cathode material for lithium-ion batteries: a first-principle study. <i>Journal of Solid State Electrochemistry</i> , 2021, 25, 1999-2007.	1.2	6
2882	Probing the effects of Al dopant over the structure and charge-related optical, magnetic, and electrical properties of Al ³⁺ -doped LaFeO ₃ bulk multiferroic materials. <i>Chemical Papers</i> , 2021, 75, 4337-4353.	1.0	4
2883	Novel Chain and Ribbon ZnO Nanoporous Crystalline Phases in Cubic Lattice. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100067.	0.7	0
2884	Thermal expansion and phase transformation in the rare earth di-titanate (<i>R</i> ₂ Ti ₂ O ₇) system. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 397-407.	0.5	3
2885	Uncertainty of exchange-correlation functionals in density functional theory calculations for lithium-based solid electrolytes on the case study of lithium phosphorus oxynitride. <i>Journal of Computational Chemistry</i> , 2021, 42, 1283-1295.	1.5	6
2886	Observing and Modeling the Sequential Pairwise Reactions that Drive Solid-State Ceramic Synthesis. <i>Advanced Materials</i> , 2021, 33, e2100312.	11.1	51
2887	Elastic Properties of the Pyrite-Type FeOOH- α -FeOOH System From First-Principles Calculations. <i>Geochemistry, Geophysics, Geosystems</i> , 2021, 22, e2021GC009703.	1.0	2
2888	Shape Control of Emissive Properties of Mn-Doped CsPbBr ₃ Nanocrystals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11462-11467.	1.5	1
2889	Combined Density Functional Theory and Microkinetics Study to Predict Optimum Operating Conditions of Si(100) Surface Carbonization by Acetylene for High Power Devices. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4558-4568.	2.1	8
2890	Phase transition, magnetic, and electronic properties of CeOInS ₂ . <i>Journal of the Ceramic Society of Japan</i> , 2021, 129, 249-253.	0.5	1
2891	Prediction of Single-Phase High-Entropy Nitrides from First-Principles Calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100140.	0.7	1
2892	Antimonene Allotropes $\hat{1}$ - and $\hat{2}$ -Phases as Promising Anchoring Materials for Lithium-Sulfur Batteries. <i>Energy & Fuels</i> , 2021, 35, 9001-9009.	2.5	15
2893	Hole Polaron Migration in Bulk Phases of TiO ₂ Using Hybrid Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12441-12450.	1.5	19
2894	Analogical discovery of disordered perovskite oxides by crystal structure information hidden in unsupervised material fingerprints. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	9
2895	Incommensurately modulated crystal structure of $\hat{1}$ - $\hat{2}$ -type sodium cobalt oxide Na _x Co ₂ O ₇ ($x \approx 0.78$). <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 371-377.	0.5	0

#	ARTICLE	IF	CITATIONS
2896	Ab-initio Calculations; Mechanical and Electronic Properties of New M4As3Co (M: Al, Ga) Compounds. SDU Journal of Science, 0, , 86-94.	0.1	0
2897	Electronic and crystal structures of $\text{LnFeAsO}_{1-x}\text{H}_x$ (Ln = La, Sm) studied by x-ray absorption spectroscopy, x-ray emission spectroscopy, and x-ray diffraction: II pressure dependence. Journal of Physics Condensed Matter, 2021, 33, 255603.	0.7	0
2898	Multiferroic ground states in free standing perovskite-based nanodots: a density functional theory study. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 055002.	0.8	1
2899	High-pressure effects on superconducting properties and crystal structure of Bi-based layered superconductor $\text{La}_2\text{O}_2\text{Bi}_3\text{Ag}_{0.6}\text{Sn}_{0.4}\text{S}_6$. Journal of Physics Condensed Matter, 2021, 33, 225702.	0.7	3
2900	Electronic structure and field emission characteristics of a new kind of BeO nanotubes: A first-principles study. Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2021, 39, 030601.	0.6	1
2901	Through-Space Charge Transfer in Copper Coordination Networks with Copper-Halide Guest Anions. Inorganic Chemistry, 2021, 60, 9273-9277.	1.9	5
2902	First Principles calculations of structural, electronic, elastic, vibrational, and thermodynamic properties of TMPs compounds (TM= Cr, Mo). Computational Condensed Matter, 2021, 27, e00541.	0.9	2
2903	Improvement of precision in refinements of structure factors using convergent-beam electron diffraction patterns taken at Bragg-excited conditions. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, 289-295.	0.0	0
2904	One-dimensional polyhedral chain of ThCl_6 encapsulated within single-walled carbon nanotubes. AIP Advances, 2021, 11, 065117.	0.6	1
2905	Atomistic insight into lithospheric conductivity revealed by phonon-electron excitations in hydrous iron-bearing silicates. Communications Materials, 2021, 2, .	2.9	8
2906	Effects of Substituting S with Cl on the Structural and Electrochemical Characteristics of Na_3SbS_4 Solid Electrolytes. ACS Applied Energy Materials, 2021, 4, 6125-6134.	2.5	28
2907	Kinetically Stabilized Cation Arrangement in Li_3YCl_6 Superionic Conductor during Solid-State Reaction. Advanced Science, 2021, 8, e2101413.	5.6	24
2908	Broadband impedance spectroscopy of $\text{Li}_4\text{Ti}_5\text{O}_{12}$: from nearly constant loss effects to long-range ion dynamics. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	0.6	4
2909	Perovskite Quantum Dot Solar Cells: An Overview of the Current Advances and Future Perspectives. Solar Rrl, 2021, 5, 2100205.	3.1	12
2910	Nonperturbative phonon scatterings and the two-channel thermal transport in Bi_2Te_3 . Physical Review B, 2021, 103, .		
2911	Site Occupation and Structural Phase Transformation of the (010) Antiphase Boundary in Boron-Modified $\text{Li}_{12}\text{Ni}_3\text{Al}$. Jom, 2021, 73, 2285-2292.	0.9	2
2912	Inclination of self-interstitial dumbbells in molybdenum and tungsten: A first-principles study. AIP Advances, 2021, 11, 065012.	0.6	3
2913	Density functional study on Am(III)/Eu(III) selectivity using crown ether type ligands. Journal of Radioanalytical and Nuclear Chemistry, 2021, 329, 77-84.	0.7	1

#	ARTICLE	IF	CITATIONS
2914	Hydrothermal Synthesis and Crystal Structure of a Novel Bismuth Oxide: $(K_{0.2}Sr_{0.8})(Na_{0.01}Ca_{0.25}Bi_{0.74})O_3$. ACS Omega, 2021, 6, 15975-15980.	1.6	11
2915	Prospects for Employing Lithium Copper Phosphates as High-Voltage Li-Ion Cathodes. Journal of Physical Chemistry C, 2021, 125, 13123-13130.	1.5	0
2916	Interplay of quantum capacitance with Van der Waals forces, intercalation, co-intercalation, and the number of MoS ₂ layers. Materials Today Energy, 2021, 20, 100677.	2.5	17
2917	New developments in the GDIS simulation package: Integration of VASP and USPEX. Journal of Computational Chemistry, 2021, 42, 1602-1626.	1.5	3
2918	Computational Insights into Molecular Adsorption Characteristics of Methylated DNA on Graphene Oxide for Multicancer Early Detection. Journal of Physical Chemistry B, 2021, 125, 6697-6708.	1.2	8
2919	Order-disorder transition of a rigid cage cation embedded in a cubic perovskite. Nature Communications, 2021, 12, 3548.	5.8	4
2920	Giant multiple caloric effects in charge transition ferrimagnet. Scientific Reports, 2021, 11, 12682.	1.6	6
2921	Terahertz and UV-VIS Spectroscopy Evaluation of Copper Doped Zinc Magnesium Titanate Nanoceramics Prepared via Sol-Gel Method. ECS Journal of Solid State Science and Technology, 2021, 10, 063007.	0.9	10
2922	Investigation of lattice anharmonicity in thermoelectric $LaO_{1-x}Bi_{2x}Se_x$ through Grüneisen parameter. Applied Physics Express, 2021, 14, 071002.	1.1	9
2923	Computationally exploring the role of S-dopant and S-linker in activating the catalytic efficiency of graphene quantum dot for ORR. Catalysis Today, 2021, 370, 36-45.	2.2	7
2924	The effects of lattice volume and carrier concentration on the conductivity of NASICON-type $LiXIn_{0.5}Zr_{0.5}(PO_4)_3$ (X = Ti, Zr; Z = Nb, Ta) oxides. Ionics, 2021, 27, 3829-3835.	1.2	1
2925	Highly Polymerized Wine-Red Carbon Nitride to Enhance Photoelectrochemical Water Splitting Performance of Hematite. Journal of Physical Chemistry C, 2021, 125, 13273-13282.	1.5	15
2926	Electronic structures and properties of TiAl/Ti ₂ AlNb heterogeneous interfaces: A comprehensive first-principles study. Intermetallics, 2021, 133, 107173.	1.8	15
2927	Type-II CeO ₂ (111)/hBN vdW heterojunction for enhanced photocatalytic hydrogen evolution: A first principles study. International Journal of Hydrogen Energy, 2021, 46, 25060-25069.	3.8	19
2928	Effect of hydrogen on the ideal shear strength in metals and its implications on plasticity: A first-principles study. International Journal of Hydrogen Energy, 2021, 46, 25726-25737.	3.8	9
2929	Substitution effect on the superconductivity in $Mo_3-xRe_xAl_2C$ with \hat{I}^2 -Mn structure prepared by microwave method*. Chinese Physics B, 2021, 30, 077401.	0.7	2
2930	Investigation on interatomic chemical bonding and charge-related optical, multiferroic properties of La ₁ Zn FeO ₃ bulk ceramics. Materials Chemistry and Physics, 2021, 267, 124652.	2.0	7
2931	Controlling the Structural Robustness of Zirconium-Based Metal Organic Frameworks for Efficient Adsorption on Tetracycline Antibiotics. Water (Switzerland), 2021, 13, 1869.	1.2	13

#	ARTICLE	IF	CITATIONS
2932	On the deactivation mechanisms of MnO ₂ electrocatalyst during operation in rechargeable zinc-air batteries studied via density functional theory. <i>Journal of Alloys and Compounds</i> , 2021, 869, 159280.	2.8	17
2933	Effect of substitution on the superconducting phase of transition metal dichalcogenide Nb(Se _x S _{3-x}) ₂ van der Waals layered structure. <i>Scientific Reports</i> , 2021, 11, 15215.	1.6	4
2934	Novel study on the electron density distribution projection maps calculated via the discrete cosine transform. <i>Journal of Applied Crystallography</i> , 2021, 54, 1198-1206.	1.9	2
2935	Titan in a Test Tube: Organic Co-crystals and Implications for Titan Mineralogy. <i>Accounts of Chemical Research</i> , 2021, 54, 3050-3059.	7.6	17
2936	Synthesis of new high-entropy alloy-type Nb ₃ (Al, Sn, Ge, Ga, Si) superconductors. <i>Journal of Alloys and Compounds</i> , 2021, 868, 159233.	2.8	21
2937	Crystal growth and physical properties of an antiferromagnetic molecule: <i>trans</i> -dibromidotetrakis(acetonitrile)chromium(III) tribromide, [CrBr ₂ (NCCH ₃) ₄](Br ₃). <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 624-631.	0.5	0
2938	Enhancing the electrochemical performance by structural evolution in O ₃ -NaFe _{1-x} Mg _x O ₂ cathodes for sodium ion batteries. <i>Inorganic Chemistry Communication</i> , 2021, 129, 108528.	1.8	6
2939	Towards high- <i>T_c</i> low-pressure superconductivity in ternary superhydrides. <i>Physical Review B</i> , 2021, 104, .	1.1	95
2940	Theoretical study of the electronic structure, magnetic and magnetocaloric properties of the DyMn ₂ O ₅ multiferroic. <i>Journal of Magnetism and Magnetic Materials</i> , 2021, 530, 167890.	1.0	5
2941	Mean inner potential of graphite measured by electron holography: Probing charge distribution and orbital diamagnetic susceptibility. <i>Carbon</i> , 2021, 179, 288-298.	5.4	6
2942	Structure-Reactivity Relationship in the High-Pressure Formation of Double-Core Carbon Nanothreads from Azobenzene Crystal. <i>Journal of Physical Chemistry C</i> , 2021, 125, 17174-17182.	1.5	13
2943	Self-learning hybrid Monte Carlo method for isothermal-isobaric ensemble: Application to liquid silica. <i>Journal of Chemical Physics</i> , 2021, 155, 034106.	1.2	6
2944	Characterization of the CaCO ₃ calcination process by the Porod invariant behaviour. <i>Journal of Applied Crystallography</i> , 2021, 54, 1127-1139.	1.9	1
2945	V ₂ CT _x MXene Artificial Solid Electrolyte Interphases toward Dendrite-Free Lithium Metal Anodes. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 9961-9969.	3.2	13
2946	Investigation of the Supramolecular Assembly of Luminescent Lanthanide Nanoparticles Surface Functionalized by Sulfonato-Calix[4]arenes with Charged Aromatic Compounds. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3761-3770.	1.0	5
2947	Electro-active properties of nanostructured films of cytosine and guanine nucleobases. <i>Nanotechnology</i> , 2021, 32, 415702.	1.3	2
2948	Influence of Reduced Na Vacancy Concentrations in the Sodium Superionic Conductors Na _{1+x} Sn ₂ P _{1-x} M _x S ₁₂ (M = Sn, Ge). <i>ACS Applied Energy Materials</i> , 2021, 4, 7250-7258.	2.5	4
2949	Synthesis and ion transport properties of RE ₃ GaO ₆ (RE = rare earth) oxide ion conductors. <i>Journal of the European Ceramic Society</i> , 2021, 41, 4516-4527.	2.8	5

#	ARTICLE	IF	CITATIONS
2950	Structural investigation and optical properties of Fe, Al, Si, and Cu ²⁺ ZnTiO ₃ nanocrystals. <i>Physica Scripta</i> , 2021, 96, 115801.	1.2	27
2951	Exomorphism of jacobsite precipitates in bixbyite single crystals from the Thomas Range in Utah. <i>American Mineralogist</i> , 2021, 106, 1163-1171.	0.9	2
2952	Stable multifunctional single-atom catalysts adsorbed on pyrazine-modified graphyne. <i>Applied Surface Science</i> , 2021, 553, 149464.	3.1	32
2953	Crystal and electronic facet analysis of ultrafine Ni ₂ P particles by solid-state NMR nanocrystallography. <i>Nature Communications</i> , 2021, 12, 4334.	5.8	17
2954	Understanding the Dependence of Nanoparticles Magnetothermal Properties on Their Size for Hyperthermia Applications: A Case Study for La-Sr Manganites. <i>Nanomaterials</i> , 2021, 11, 1826.	1.9	21
2955	Relation between crystal structure and lattice oxygen content of sintered reaction-bonded silicon nitride. <i>Journal of the American Ceramic Society</i> , 2021, 104, 6563.	1.9	2
2956	Anisotropic superconductivity in the topological crystalline metal $Pb_{1-x}Ta_xS_2$ with multiple Dirac fermions. <i>Physical Review B</i> , 2021, 104, .	1.1	5
2957	Quasi-1D XY antiferromagnet Sr ₂ Ni(SeO ₃) ₂ Cl ₂ at Sakai-Takahashi phase diagram. <i>Scientific Reports</i> , 2021, 11, 15002.	1.6	1
2958	Density Functional Theory Study of the Structure of the Pillared Hofmann Compound Ni(3-Methyl-4,4'-bipyridine)[Ni(CN) ₄] (Ni-BpyMe or PICNIC-21). <i>Journal of Physical Chemistry C</i> , 2021, 125, 15882-15889.	1.5	3
2959	Borophene via Micromechanical Exfoliation. <i>Advanced Materials</i> , 2021, 33, e2102039.	11.1	56
2960	Structural, vibrational, optical, dielectric, and shielding characteristics of (1-x)Mg(Ti _{0.95} Sn _{0.05})O ₃ -(x)SrTiO ₃ (0 ≤ x ≤ 0.1) ceramics. <i>Materials Research Bulletin</i> , 2021, 139, 111245.	2.7	6
2961	Green synthesis of LaCrO ₃ powder mediated by the extract of the Amazon rainforest native plant <i>Himatanthus drasticus</i> (Mart.) Plumel and their photocatalytic activity. <i>Journal of Materials Research and Technology</i> , 2021, 13, 2006-2011.	2.6	5
2962	Strain induced second-order Jahn-Teller reconstruction and magnetic moment modulation at monovacancy in graphene. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	7
2963	Tutorial on Chemical Pressure Analysis: How Atomic Packing Drives Laves/Zintl Intergrowth in K ₃ Au ₅ Tl. <i>Crystals</i> , 2021, 11, 906.	1.0	12
2964	A new type of cuprous-cysteamine sensitizers: Synthesis, optical properties and potential applications. <i>Materials Today Physics</i> , 2021, 19, 100435.	2.9	12
2965	High Thermal Conductivity of Wurtzite Boron Arsenide Predicted by Including Four-Phonon Scattering with Machine Learning Potential. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 53409-53415.	4.0	26
2966	Exploring the structure of atom-precise silver-palladium bimetallic clusters prepared via improved single-pot co-reduction synthesis protocol. <i>Journal of Chemical Physics</i> , 2021, 155, 084301.	1.2	4
2967	Comparative study on the strain-dependent mechanical and electronic properties of Nb ₃ Al and Nb ₃ Sn. <i>Materials Research Express</i> , 2021, 8, 086001.	0.8	4

#	ARTICLE	IF	CITATIONS
2968	Microcrystal-Induced Crystallization Effect for High-Quality Germanium/Silicon Heteroepitaxial Nanofilms. ACS Applied Electronic Materials, 2021, 3, 3391-3399.	2.0	4
2969	Two-Dimensional Janus FeXY (X, Y = Cl, Br, and I, X ≠ Y) Monolayers: Half-Metallic Ferromagnets with Tunable Magnetic Properties under Strain. ACS Applied Materials & Interfaces, 2021, 13, 38897-38905.	4.0	84
2970	A comparative study of CO catalytic oxidation on the single vacancy and di-vacancy graphene supported single-atom iridium catalysts: A DFT analysis. Surfaces and Interfaces, 2021, 25, 101293.	1.5	40
2971	Effects of Pore Connectivity on the Sorption of Fluids in Nanoporous Material: Ethane and CO ₂ Sorption in Silicalite. ChemEngineering, 2021, 5, 55.	1.0	5
2972	Cerium based UiO-66 MOF as a multipollutant adsorbent for universal water purification. Journal of Hazardous Materials, 2021, 416, 125941.	6.5	168
2973	Growth of SrB ₄ O ₇ Crystal Fibers along the c-Axis by Micro-Pulling-Down Method. Crystals, 2021, 11, 987.	1.0	1
2974	Neutron Scattering Study on Yttrium Iron Garnet for Spintronics. Journal of the Physical Society of Japan, 2021, 90, 081002.	0.7	3
2975	Switching of antiferromagnetic states in LiCoPO_4 as investigated via the magnetoelectric effect. Physical Review B, 2021, 104, .		4
2976	Roles of Polymerized Anionic Clusters Stimulating for Hydrolysis Deterioration in $\text{Li}_7\text{P}_3\text{S}_{11}$. Journal of Physical Chemistry C, 2021, 125, 19509-19516.	1.5	10
2977	Conversion of methane to methanol on C-doped boron nitride: A DFT study. Computational and Theoretical Chemistry, 2021, 1202, 113291.	1.1	8
2978	Syntheses of Novel Coordination Polymers Using Bis-Imidazole Ligand Having Steric Hindrance and Methoxy Group. Trends Journal of Sciences Research, 2021, 1, 29-37.	0.0	1
2979	Density Functional Theory Study on the ¹⁹³ Ir Mössbauer Spectroscopic Parameters of Vaska's Complexes and Their Oxidative Adducts. Inorganic Chemistry, 2021, 60, 12740-12752.	1.9	3
2980	Observation of Giant Optical Linear Dichroism in a Zigzag Antiferromagnet FePS ₃ . Nano Letters, 2021, 21, 6938-6945.	4.5	37
2981	Crystal-Site-Based Artificial Neural Networks for Material Classification. Crystals, 2021, 11, 1039.	1.0	3
2982	The Impact of Vibrational Entropy on the Segregation of Cu to Antiphase Boundaries in Fe ₃ Al. Magnetochemistry, 2021, 7, 108.	1.0	3
2983	(INVITED) Revisiting Duffy's model for Sb ³⁺ and Bi ³⁺ in double halide perovskites: Emergence of a descriptor for machine learning. Optical Materials: X, 2021, 11, 100082.	0.3	2
2984	Multifold Electrochemical Protons and Zinc Ion Storage Behavior in Copper Vanadate Cathodes. ACS Applied Energy Materials, 2021, 4, 10197-10202.	2.5	4
2985	Extremely flat band in antiferroelectric bilayer In_2Se_3 with large twist-angle. New Journal of Physics, 2021, 23, 083019.	1.2	11

#	ARTICLE	IF	CITATIONS
2986	Catalytic Functionalization of Hexagonal Boron Nitride for Oxidation and Epoxidation Reactions by Molecular Oxygen. <i>Journal of Physical Chemistry C</i> , 2021, 125, 19219-19228.	1.5	2
2987	Oxygen-Defect Enhanced Anion Adsorption Energy Toward Super-Rate and Durable Cathode for Ni ²⁺ /Zn Batteries. <i>Nano-Micro Letters</i> , 2021, 13, 167.	14.4	52
2988	Unravelling the ion-energy-dependent structure evolution and its implications for the elastic properties of (V,Al)N thin films. <i>Acta Materialia</i> , 2021, 214, 117003.	3.8	20
2989	The effect of Na addition on the first hydrogen absorption kinetics of cast hypoeutectic Mg ²⁺ /La alloys. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 27096-27106.	3.8	10
2990	Multifunctionality in (K,Na)NbO ₃ -based ceramic near polymorphic phase boundary. <i>Journal of Applied Physics</i> , 2021, 130, 064102.	1.1	2
2991	Band Gap Engineering and 14 Electron Superatoms in 2D Superoctahedral Boranes B ₄ X ₂ (B, N, P, As, Sb). <i>Journal of Physical Chemistry C</i> , 2021, 125, 17280-17290.	1.5	6
2992	Defect Polaritons from First Principles. <i>ACS Nano</i> , 2021, 15, 15142-15152.	7.3	7
2993	High-temperature superconductor of sodalite-like clathrate hafnium hexahydride. <i>Scientific Reports</i> , 2021, 11, 16403.	1.6	9
2994	Mechanism and Effect of the Dilution Gas Flow Rate on Various Fe ²⁺ /Si/SiO ₂ Soft Magnetic Composites during Fluidised Bed Chemical Vapour Deposition. <i>Crystals</i> , 2021, 11, 963.	1.0	3
2995	Outstanding Catalytic Effects of 1T ⁺ -MoTe ₂ Quantum Dots@3D Graphene in Shuttle-Free Li ⁺ /S Batteries. <i>ACS Nano</i> , 2021, 15, 13279-13288.	7.3	81
2996	In-plane magnetic structure and exchange interactions in the high-temperature antiferromagnet Cr ₂ Al. <i>Physical Review Materials</i> , 2021, 5, .	0.9	1
2997	Torsional strain engineering of transition metal dichalcogenide nanotubes: an ab initio study. <i>Nanotechnology</i> , 2021, 32, 47LT01.	1.3	9
2998	Theoretical study on the tunable electronic band structure of Cs ₂ PbI ₂ Cl ₂ /CsPbBr ₃ halide perovskite heterostructure driven by ferroelectric polarization modulation. <i>Journal of Colloid and Interface Science</i> , 2021, 597, 233-241.	5.0	14
2999	A First-Principles Investigation on Electronic Structure, Optical and Thermoelectric Properties of Janus In ₂ SeTe Monolayer. <i>Journal of Superconductivity and Novel Magnetism</i> , 2021, 34, 3279-3290.	0.8	23
3000	Controlling the Shape Anisotropy of Monoclinic Nb ₁₂ O ₂₉ Nanocrystals Enables Tunable Electrochromic Spectral Range. <i>Journal of the American Chemical Society</i> , 2021, 143, 15745-15755.	6.6	23
3001	A Comparison of Order-Disorder in Several Families of Cubic Oxides. <i>Frontiers in Chemistry</i> , 2021, 9, 719169.	1.8	5
3002	Achievement of strain-driven ultrahigh carrier mobility in $\hat{1}^2$ -TeO ₂ . <i>Materials Research Bulletin</i> , 2021, 141, 111343.	2.7	5
3003	Electric-field modulated photovoltaic effect of ferroelectric double-perovskite Bi ₂ FeMnO ₆ films. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	7

#	ARTICLE	IF	CITATIONS
3004	Role of H impurity as compensating center in BiFeO ₃ by first-principle calculations. Physica Scripta, 2021, 96, 125813.	1.2	0
3005	Course on the Use of DFT Calculations to Improve Understanding of Phase Diagrams in Solid-State Chemistry. Journal of Chemical Education, 2021, 98, 3207-3217.	1.1	2
3006	Theoretical investigation of metal oxides for SO ₂ capture through first-principles calculations. International Journal of Quantum Chemistry, 0, , e26822.	1.0	1
3007	High CO ₂ resistance of indium-doped cobalt-free 60Åwt.%Ce0.9Pr0.1O ₂ -40Åwt.%Pr0.6Sr0.4Fe1-In O ₃ oxygen transport membranes. Ceramics International, 2022, 48, 415-426.	2.3	10
3008	Phototribology: Control of Friction by Light. ACS Applied Materials & Interfaces, 2021, 13, 43746-43754.	4.0	5
3009	Ab initio study of the structure and relative stability of MgSiO ₄ H ₂ polymorphs at high pressures and temperatures. American Mineralogist, 2022, 107, 781-789.	0.9	2
3010	Structural effects on the emission dynamics of oxide crystals activated with Tb ³⁺ . Journal of Solid State Chemistry, 2021, 301, 122306.	1.4	1
3012	Unravelling the crystal structure and optoelectronic properties of C ₃ H ₃ M ₃ (M = Sn, Pb) for solar cell applications. Solar Energy Materials and Solar Cells, 2021, 230, 111133.	3.0	1
3013	Optical, Electrochemical, and Photoelectrochemical Behavior of Copper Pyrovanadate: A Unified Theoretical and Experimental Study. Journal of Physical Chemistry C, 2021, 125, 19609-19620.	1.5	4
3014	Catalyzing Bond Dissociation in Graphene via Alkali Iodide Molecules. Small, 2021, 17, e2102037.	5.2	1
3015	How Li diffusion in spinel Li[Ni _{1/2} Mn _{3/2}]O ₄ is seen with $\langle i \rangle^{1/4} \langle i \rangle^{\sup \text{Å} \pm \sup} \text{SR}$. Zeitschrift Fur Physikalische Chemie, 2022, 236, 799-816.	1.4	5
3016	Approaches to modelling the shape of nanocrystals. Nano Convergence, 2021, 8, 26.	6.3	22
3017	Comparative Studies of the Structural and Transport Properties of Molten Salt FLiNaK Using the Machine-Learned Neural Network and Reparametrized Classical Forcefields. Journal of Physical Chemistry B, 2021, 125, 10562-10570.	1.2	19
3018	Structural Investigation into Magnetic Spin Orders of a Manganese Phosphatic Oxyhydroxide, Mn ₅ [(PO ₄) ₂ (PO ₃ (OH)) ₂](HOH) ₄ . Symmetry, 2021, 13, 1688.	1.1	1
3019	Anomalous broadening of specific heat jump at T _c in high-entropy-alloy-type superconductor TrZr ₂ . Superconductor Science and Technology, 0, , .	1.8	12
3020	High oxygen permeation flux of cobalt-free Cu-based ceramic dual-phase membranes. Journal of Membrane Science, 2021, 633, 119403.	4.1	17
3021	Mechanisms behind high CO ₂ /CH ₄ selectivity using ZIF-8 metal organic frameworks with encapsulated ionic liquids: A computational study. Chemical Engineering Journal, 2021, 419, 129638.	6.6	19
3022	Enhanced Photocatalytic Activity in Strain Engineered Janus WSSe Monolayers. Journal of Electronic Materials, 2021, 50, 7230-7239.	1.0	7

#	ARTICLE	IF	CITATIONS
3023	Lessons learned from FeSb ₂ O ₄ on stereoactive lone pairs as a design principle for anion insertion. Cell Reports Physical Science, 2021, 2, 100592.	2.8	3
3024	Olefin-linked covalent organic frameworks with twisted tertiary amine knots for enhanced ultraviolet detection. Chinese Chemical Letters, 2022, 33, 2621-2624.	4.8	7
3025	Radiative properties of $\text{Li}^{2+}\text{Al}^{3+}\text{Si}^{4+}\text{O}$ ceramics: Effect of Li^{2+} to Al^{3+} ratio. Ceramics International, 2021, 48, 278-278.	2.3	0
3026	Evaluation of electron currents from cesium-coated tungsten emitter arrays with inclusion of space charge effects, workfunction changes, and screening. Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, 2021, 39, .	0.6	3
3028	Crystal Structure Evolution of UCl ₃ from Room Temperature to Melting. Jom, 2021, 73, 3555-3563.	0.9	5
3029	Semiconducting phase of hafnium dioxide under high pressure: a theoretical studied by quasi-particle GW calculations. Materials Research Express, 0, , .	0.8	3
3030	Roles of oxygen-containing functional groups of O-doped g-C ₃ N ₄ in catalytic ozonation: Quantitative relationship and first-principles investigation. Applied Catalysis B: Environmental, 2021, 292, 120155.	10.8	137
3031	Non-magnetic ions doping effects in the magnetic properties of zircon-type GdCrO ₄ compound. Journal of Magnetism and Magnetic Materials, 2021, 533, 167953.	1.0	2
3032	Mechanisms and thermodynamic modelling of iodide sorption on AFm phases. Journal of Colloid and Interface Science, 2022, 608, 683-691.	5.0	7
3033	Experimental overview on pairing mechanisms of BiCh ₂ -based (Ch: S, Se) layered superconductors. Journal of Physics Condensed Matter, 2021, 33, 473001.	0.7	7
3034	Theoretical study on near UV and visible optical absorption characteristics of Ti-doped Al_2O_3 single crystals. Materials Today Communications, 2021, 28, 102506.	0.9	4
3035	Identifying Migration Channels and Bottlenecks in Monoclinic NASICON-type Solid Electrolytes with Hierarchical Ion Transport Algorithms. Advanced Functional Materials, 2021, 31, 2107747.	7.8	33
3036	Modulating electronic, magnetic and mechanical properties of MVN (M = Ti, V, Cr) MXenes by surface functionalization. Solid State Communications, 2021, 336, 114411.	0.9	7
3037	Sensitive H ₂ gas sensors based on SnO ₂ nanowires. Sensors and Actuators B: Chemical, 2021, 345, 130334.	4.0	82
3038	Doping effect of Cu (II) in the adsorption of CrO ₄ ²⁻ by the Fe ₃ O ₄ (1 1 1) surface: A theoretical study. Chemical Physics Letters, 2021, 781, 138984.	1.2	6
3039	Investigation into thermoelectric properties of M (M=Hf, Zr) X ₂ (X=S, Se, Te) nanotubes using first-principles calculation. Solid State Communications, 2021, 336, 114289.	0.9	9
3040	Bi-atom active sites embedded in a two-dimensional covalent organic framework for efficient nitrogen reduction reaction. Applied Surface Science, 2021, 563, 150352.	3.1	25
3041	Ab initio investigation of physical properties of the graphene/As-F hetero-bilayer. Applied Surface Science, 2021, 563, 150339.	3.1	6

#	ARTICLE	IF	CITATIONS
3042	Hierarchical flower-like TiO ₂ microspheres for high-selective NH ₃ detection: A density functional theory study. <i>Sensors and Actuators B: Chemical</i> , 2021, 345, 130303.	4.0	27
3043	Substantial role of charge transfer on the diffusion mechanism of interstitial elements in δ -titanium: A First-principles study. <i>Scripta Materialia</i> , 2021, 203, 114065.	2.6	12
3044	Selective oxidation of thermoelectric TiNiSn. <i>Computational Materials Science</i> , 2021, 198, 110682.	1.4	1
3045	Ni diffusion in ceria lattice: A combined experimental and theoretical study. <i>Acta Materialia</i> , 2021, 219, 117252.	3.8	9
3046	Excited state dynamics in monolayer black phosphorus revisited: Accounting for many-body effects. <i>Journal of Chemical Physics</i> , 2021, 155, 134106.	1.2	13
3047	A Cr ^{1/4} neisen tensor for rutile and its application to host-inclusion systems. <i>American Mineralogist</i> , 2021, 106, 1586-1595.	0.9	6
3048	Raman scattering and Cr ³⁺ luminescence study on the structural behavior of β -AlOOH at high pressures. <i>American Mineralogist</i> , 2021, , .	0.9	0
3049	Mutual transformation of reversible and bound polarization in Y-type BaSrCo ₂ Fe ₁₁ AlO ₂₂ ceramics. <i>Ceramics International</i> , 2021, 47, 32445-32449.	2.3	4
3050	Ultralow and glass-like lattice thermal conductivity in crystalline BaAg ₂ Te ₂ : Strong fourth-order anharmonicity and crucial diffusive thermal transport. <i>Materials Today Physics</i> , 2021, 21, 100487.	2.9	17
3051	High fluoride-ion conductivity and fluoride-ion conductor \hat{w} insulator transition in fluorinated hexagonal boron nitride. <i>Materials Today Physics</i> , 2021, 21, 100523.	2.9	1
3052	Superconductivity of centrosymmetric and non-centrosymmetric phases in antiperovskite (Ca,Sr)Pd ₃ P. <i>Journal of Alloys and Compounds</i> , 2021, 882, 160733.	2.8	6
3053	In-situ exsolution of Ni nanoparticles to achieve an active and stable solid oxide fuel cell anode catalyst on A-site deficient La _{0.4} Sr _{0.4} Ti _{0.94} Ni _{0.06} O _{3-δ} . <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 103, 264-274.	2.9	17
3054	Density functional theory study on the role of ternary alloying elements in TiFe-based hydrogen storage alloys. <i>Journal of Materials Science and Technology</i> , 2021, 92, 148-158.	5.6	25
3055	Interfacial strain relief by periodic dislocation doublets arising from rotationally related orientation relationships of Y ₄ Zr ₃ O ₁₂ dispersions in ferrite matrix. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2021, 828, 142047.	2.6	4
3056	Nature of electronic topological transition and superconductivity in bismuth under high pressure from ab initio random structure searching. <i>Computational Materials Science</i> , 2021, 200, 110806.	1.4	5
3057	Borderline first-order magnetic phase transition in AlFe ₂ B ₂ . <i>Journal of Alloys and Compounds</i> , 2021, 886, 161150.	2.8	4
3058	Li ₂ Ni(WO ₄) ₂ /C: A potential tungstate anode material for lithium ion batteries. <i>Journal of Alloys and Compounds</i> , 2021, 888, 161535.	2.8	3
3059	Two-dimensional PtSe ₂ /hBN vdW heterojunction as photoelectrocatalyst for the solar-driven oxygen evolution reaction: A first principles study. <i>Applied Surface Science</i> , 2021, 570, 151207.	3.1	24

#	ARTICLE	IF	CITATIONS
3060	Two-dimensional hetero-nanostructured electrocatalyst of Ni/NiFe-layered double oxide for highly efficient hydrogen evolution reaction in alkaline medium. <i>Chemical Engineering Journal</i> , 2021, 426, 131827.	6.6	42
3061	Probing on crystallographic structural and surface morphology of hydrothermally synthesized MoS ₂ nanoflowers consisting of nanosheets. <i>Applied Surface Science Advances</i> , 2021, 6, 100167.	2.9	11
3062	Extremely intense green up-conversion luminescent and ultra-high temperature sensitivity in Er ³⁺ /Yb ³⁺ co-doped BiTa ₇ O ₁₉ phosphors. <i>Journal of Luminescence</i> , 2022, 241, 118484.	1.5	24
3063	Enabling photocatalytic hydrogen production over Fe-based MOFs by refining band structure with dye sensitization. <i>Chemical Engineering Journal</i> , 2022, 429, 132217.	6.6	29
3064	Metamagnetic transitions induced by doping with non-magnetic 4d ions in ludwigites Co ₅ A(O ₂ BO ₃) ₂ (A=Zr and Hf). <i>Journal of Alloys and Compounds</i> , 2022, 890, 161717.	2.8	4
3065	Hydrogen-induced tunable electronic and optical properties of a two-dimensional penta-Pt ₂ N ₄ monolayer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10409-10417.	1.3	24
3066	Predicting activation energies for vacancy-mediated diffusion in alloys using a transition-state cluster expansion. <i>Physical Review Materials</i> , 2021, 5, .	0.9	7
3067	Assessing Nickel Titanium Binary Systems Using Structural Search Methods and Ab Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1578-1591.	1.5	3
3068	Pressure Induced Hydrogen Order-Disorder Transition in β -Ni(OH) ₂ . <i>Journal of Physical Chemistry C</i> , 2021, 125, 2785-2792.	1.5	7
3069	An efficient implementation of spin-orbit coupling within the framework of semiempirical orthogonalization-corrected methods for ultrafast intersystem crossing dynamics. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22313-22323.	1.3	4
3070	Strain effects on band structure and Dirac nodal-line morphology of ZrSiSe. <i>Journal of Applied Physics</i> , 2021, 129, .	1.1	3
3071	Anisotropic Structural Collapse of Mg ₃ Sb ₂ and Mg ₃ Bi ₂ at High Pressure. <i>Chemistry of Materials</i> , 2021, 33, 567-573.	3.2	14
3072	Raman analysis and crystal structure of polycrystalline LiNi _{1-x} CoxPO ₄ (x=0-0.5). <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	1.1	2
3073	First-principles study of the morphology and surface structure of La _{0.5} Sr _{0.5} Fe _{0.5} Co _{0.5} O ₃ perovskites as air electrodes for solid oxide fuel cells. <i>Science and Technology of Advanced Materials Methods</i> , 2021, 1, 24-33.	0.4	1
3074	Thermal enhancement of the ² H _{11/2} → ⁴ I _{15/2} up-conversion luminescence of Er ³⁺ -doped K ₂ Yb(PO ₄) ₄ (MoO ₄) phosphors. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12159-12167.	2.7	12
3075	Computational mining of Janus Sc ₂ C-based MXenes for spintronic, photocatalytic, and solar cell applications. <i>Journal of Materials Chemistry A</i> , 2021, 9, 10882-10892.	5.2	52
3076	Electronic and thermodynamic properties of native point defects in V ₂ O ₅ : a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11374-11387.	1.3	18
3077	A decomposition mechanism for Mn ₂ (DSBDC) metal-organic frameworks in the presence of water molecules. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22794-22803.	1.3	2

#	ARTICLE	IF	CITATIONS
3078	Engineering the electronic band structure and thermoelectric performance of GeTe <i>via</i> lattice structure manipulation from first-principles. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23576-23585.	1.3	6
3080	Lanthanum-Based Perovskites for Catalytic Oxygen Evolution Reaction. <i>ChemElectroChem</i> , 2020, 7, 3173-3192.	1.7	50
3081	Bonding Environments in a Creep-Resistant Mg-RE-Zn Alloy. <i>Minerals, Metals and Materials Series</i> , 2017, , 471-475.	0.3	3
3082	Binary and Ternary Random Alloys. <i>Springer Series in Optical Sciences</i> , 2015, , 29-47.	0.5	4
3083	A general perspective of Fe-Mn-Al-C steels. <i>Journal of Materials Science</i> , 2018, 53, 14003-14062.	1.7	148
3084	Fabrication and luminescence of Ca ₂ LaTaO ₆ :RE ³⁺ (RE = Sm, Eu and Pr) phosphors. <i>Chemical Physics Letters</i> , 2020, 758, 137923.	1.2	3
3085	The investigation of electronic, anisotropic elastic and lattice dynamical properties of MAB phase nanolaminated ternary borides: $M_{2}AlB_{2}$		

#	ARTICLE	IF	CITATIONS
3097	Superconductivity of superhydride CeH ₁₀ under high pressure. Materials Research Express, 2020, 7, 086001.	0.8	26
3098	Two-fold symmetry of in-plane magnetoresistance anisotropy in the superconducting states of BiCh ₂ -based LaO _{0.9} F _{0.1} BiSe single crystal. Journal of Physics Communications, 2020, 4, 095028.	0.5	11
3099	A combined density functional theory and x-ray photoelectron spectroscopy study of the aromatic amino acids. Electronic Structure, 2020, 2, 044005.	1.0	11
3100	Relationship between magnetic ordering and gigantic magnetocaloric effect in HoB ₂ studied by neutron diffraction experiment. Physical Review B, 2020, 102, .	1.1	7
3101	Spin Jahn-Teller antiferromagnetism in $\text{CoTiMn}_2\text{O}_5$. Physical Review B, 2019, 99, .	1.1	10
3102	Mechanical properties and phase stability of monoborides using density functional theory calculations. Physical Review Materials, 2017, 1, .	0.9	4
3103	Experimental and first-principles calculation study of the pressure-induced transitions to a metastable phase in GaPO ₄ and in the solid solution AlPO ₄ ^x GaPO ₄ . Physical Review Materials, 2017, 1, .	0.9	3
3104	Pressure-stabilized binary compounds of magnesium and silicon. Physical Review Materials, 2018, 2, .	0.9	13
3105	Octahedral tilting instabilities in inorganic halide perovskites. Physical Review Materials, 2018, 2, .	0.9	73
3106	First-principles thermodynamics study of phase stability in inorganic halide perovskite solid solutions. Physical Review Materials, 2018, 2, .	0.9	27
3107	Quantum-mechanical process of carbonate complex formation and large-scale anisotropy in the adsorption energy of CO_2 on anatase TiO_2 .	0.9	9
3108	Two-dimensional silicon boride on ZrB ₂ . Physical Review Materials, 2019, 3, .	0.9	50
3109	Anomalous Hall conductivity of noncollinear magnetic antiperovskites. Physical Review Materials, 2019, 3, .	0.9	50
3110	Hidden kagome-lattice picture and origin of high conductivity in delafossite PtCoO_2 . Physical Review Materials, 2019, 3, .	0.9	10
3111	Frank-Turnbull dopant migration may enhance heteroatom diffusivity: Evidence from alkali-doped Cu(In,Ga)Se ₂ . Physical Review Materials, 2019, 3, .	0.9	10
3112	Magnetic moment of rare-earth elements in R_2B_2 estimated with structural disorder and magnetic correlations driven by oxygen doping in R_2NiO_3 .	0.9	6
3113	Structural disorder and magnetic correlations driven by oxygen doping in R_2NiO_3 .	0.9	6

#	ARTICLE	IF	CITATIONS
3115	Superconductivity induced by Mg deficiency in noncentrosymmetric phosphide $\langle \text{mml:math} \text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{Mg} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{Rh} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{P} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$. Physical Review Materials, 2019, 3, .	0.9	11
3116	Anharmonicity measure for materials. Physical Review Materials, 2020, 4, .	0.9	45
3117	<i>Ab initio</i> study of chemical disorder as an effective stabilizing mechanism of bcc-based $\langle \text{mml:math} \text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mi} \rangle \text{TiAl} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle$	0.9	2
3118	$\langle \text{mml:math} \text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{Bi} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{Se} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ thin films heteroepitaxially grown on $\langle \text{mml:math} \text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \hat{\text{I}} \langle \text{mml:mi} \rangle \langle \text{mml:mtext} \rangle \hat{\text{a}}^{\text{r}} \langle \text{mml:mtext} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{Li} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \text{Mn} \langle \text{mml:mi} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{P} \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \text{mathvariant}=\text{"normal"} \rangle \text{O} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 4 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$ lithium diffusion in $\langle \text{mml:math} \text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:mi} \rangle \hat{\text{I}}^{4} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle \hat{\text{A}}_{\pm} \langle \text{mml:mo} \rangle \langle \text{mml:msup} \rangle \langle \text{mml:mi} \rangle$	0.9	2
3119	Rietveld refinement of Sr ₅ (AsO ₄) ₃ Cl from high-resolution synchrotron data. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, i16-i17.	1.3	15
3120	RbCa ₂ Nb ₃ O ₁₀ from X-ray powder data. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, i44-i44.	0.2	4
3121	RbCa ₂ Nb ₃ O ₁₀ from X-ray powder data. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, i44-i44.	0.2	8
3122	Expression and interactions of stereochemically active lone pairs and their relation to structural distortions and thermal conductivity. IUCrJ, 2020, 7, 480-489.	1.0	18
3123	Structural elucidation of triclinic and monoclinic SFCA-III $\hat{\text{a}}^{\text{c}}$ killing two birds with one stone. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 1126-1136.	0.5	14
3124	Rietveld refinement of the crystal structures of Rb ₂ X ₅ Si ₅ O ₁₂ (X = Ni, Mn). Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 249-252.	0.2	5
3125	Betaine (trimethylammonioacetate) binary compound with sodium iodide. IUCrData, 2018, 3, .	0.1	1
3126	Chemical vapor deposition route to transparent thick films of Eu ³⁺ -doped HfO ₂ and Lu ₂ O ₃ for luminescent phosphors. Optical Materials Express, 2020, 10, 899.	1.6	13
3127	First-principle Calculations of Dopant-Oxygen Vacancy Complexes in Transparent Conducting TiO ₂ Systems. Hyomen Kagaku, 2010, 31, 343-351.	0.0	3
3128	Synthesis and ionic conductivity of a high-entropy layered hydroxide. Journal of the Ceramic Society of Japan, 2020, 128, 336-339.	0.5	13
3129	Hydrothermal synthesis and crystal structure of a mixed-valence pyrochlore-type strontium bismuthate, (Sr _{0.75} Bi _{0.25}) ₂ Bi ₂ O _{6.83} . Journal of the Ceramic Society of Japan, 2020, 128, 660-663.	0.5	3
3130	Phase transitions in $\hat{\mu}$ -FeOOH at high pressure and ambient temperature. American Mineralogist, 2020, 105, 1769-1777.	0.9	20
3131	Sursassite: Hydrogen bonding, cation order, and pumpellyite intergrowth. American Mineralogist, 2009, 94, 1440-1449.	0.9	9
3132	Charge Density of Al Doped Lanthanum Orthoferrites. Materials Research Foundations, 2016, , 108-127.	0.2	2

#	ARTICLE	IF	CITATIONS
3134	Structure prediction and energy landscape exploration in the zinc oxide system. Processing and Application of Ceramics, 2011, 5, 73-78.	0.4	15
3135	Identification of promising chemical systems for the synthesis of new materials structure types: An ab initio minimization data mining approach. Processing and Application of Ceramics, 2013, 7, 37-41.	0.4	12
3136	Pumpellyite-, sursassite-, and epidote-type structures: common principles-individual features. Journal of Mineralogical and Petrological Sciences, 2011, 106, 211-222.	0.4	2
3137	Interlayer Bonding Energy of Mg-Chlorite: A Density Functional Theory Study. Journal of Computer Chemistry Japan, 2015, 14, 152-154.	0.0	4
3138	Ferroelectricity of Dionâ€“Jacobson layered perovskites CsNdNb ₂ O ₇ and RbNdNb ₂ O ₇ . Japanese Journal of Applied Physics, 2020, 59, SPPC04.	0.8	12
3139	Charge order of bismuth ions and nature of chemical bonds in double perovskite-type oxide BaBiO ₃ visualized by synchrotron radiation X-ray diffraction. Japanese Journal of Applied Physics, 2020, 59, 095505.	0.8	2
3140	Unconventional isotope effect on transition temperature in BiS ₂ -based superconductor Bi ₄ O ₄ S ₃ . Applied Physics Express, 2020, 13, 093001.	1.1	12
3141	High thermal stable blue-emitting alkali silicate phosphor, Eu ²⁺ -activated Na ₂ Mg ₂ Si ₆ O ₁₅ . Journal of Ceramic Processing Research, 2019, 20, 205-210.	0.4	1
3142	Proton Conduction in Nonstoichiometric λ -3 BaZrO ₃ (210)[001] Tilt Grain Boundary Using Density Functional Theory. Journal of the Korean Ceramic Society, 2016, 53, 301-305.	1.1	5
3143	Synthesis, Structural and Photophysical Properties of Gd ₂ O ₃ :Eu ³⁺ Nanostructures Prepared by a Microwave Sintering Process. Advances in Chemical Engineering and Science, 2014, 04, 374-388.	0.52	22
3144	Fabrication, Optoelectronic and Photocatalytic Properties of Some Composite Oxide Nanostructures. Transactions on Electrical and Electronic Materials, 2010, 11, 1-10.	1.0	20
3146	Crystal Structures of Luminescent Oxyborates. Nihon Kessho Gakkaishi, 2012, 54, 68-73.	0.0	3
3147	Quaternary sulphides Cu ₂ Zn(Ti, Zr, Hf)S ₄ , the new type of photovoltaic materials. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 068801.	0.2	1
3148	Synthesis of New Layered Oxypnictides Sr ₂ CrO ₂ (FeAs) ₂ . Journal of the Physical Society of Japan, 2013, 82, 045002.	0.7	10
3149	Preparation and Thermoelectric Properties of a Chimney-Ladder (Mn _{1-x} Fe _x)Si ₃ ($\hat{1}\hat{3}\hat{1}\hat{7}$) Solid Solution. Japanese Journal of Applied Physics, 2011, 50, 035804.	0.8	26
3150	High-Temperature Thermoelectric Property of Layered La _{2-2x} Ca _{1+2x} Mn ₂ O ₇ Manganites (0.75) Tj ETQ@1&l 0.784&3 14 rgB	0.784	14
3151	Comparative Study of Multiplet Structures of Mn ⁴⁺ in K ₂ SiF ₆ , K ₂ GeF ₆ , and K ₂ TiF ₆ Based on First-Principles Configurationâ€“Interaction Calculations. Japanese Journal of Applied Physics, 2012, 51, 022604.	0.8	9
3152	Enhanced Thermoelectric Performance of a Chimney-Ladder (Mn _{1-x} Crx)Si ₃ ($\hat{1}\hat{3}\hat{1}\hat{7}$) Solid Solution. Japanese Journal of Applied Physics, 2012, 51, 085801.	0.8	9

#	ARTICLE	IF	CITATIONS
3171	Age-hardening structure and mechanism of Cu ³ Ni ^{1.5} Si Corson alloy. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2022, 831, 142220.	2.6	13
3172	Chirality and Magnetocaloricity in GdFeTeO ₆ as Compared to GdGaTeO ₆ . <i>Materials</i> , 2021, 14, 5954.	1.3	2
3173	Synthesis and Ion-Transport Properties of EuKGe ₂ O ₆ -, Ca ₃ Fe ₂ Ge ₃ O ₁₂ -, and BaCu ₂ Ge ₂ O ₇ -Type Oxide-Ion Conductors. <i>Inorganic Chemistry</i> , 2021, 60, 17019-17032.	1.9	1
3174	Effects of Bi Substitution on the Cobalt-Free 60wt.%Ce _{0.9} Pr _{0.1} O ₂ -40wt.%Pr _{0.6} Sr _{0.4} Fe _{1-x} BixO ₃ Oxygen Transport Membranes. <i>Processes</i> , 2021, 9, 1767.	1.3	4
3175	In situ synchrotron radiation X-ray diffraction measurements of Fe-Mo alloy hydrides formed under high pressure and high temperature. <i>Journal of Alloys and Compounds</i> , 2022, 893, 162300.	2.8	4
3176	Computational study of electronic properties of X-doped hexagonal boron nitride (h-BN): X=(Li, Be, Al). <i>TiEJQq110.78431</i>	0.8	4
3177	Molecular Dynamics Simulation of Li-Ion Conduction at Grain Boundaries in NASICON-Type Li ₂ (PO ₄) ₃ Solid Electrolytes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 23604-23612.	1.5	14
3178	Phase-Controllable Synthesis of Multifunctional 1T-MoSe ₂ Nanostructures: Applications in Lithium-Ion Batteries, Electrocatalytic Hydrogen Evolution, and the Hydrogenation Reaction. <i>ChemElectroChem</i> , 2021, 8, 4148-4155.	1.7	4
3179	Luminescent core-shell Ca ₂ MoO ₅ :Eu ³⁺ -MCM-41 structure for sustained drug release. <i>Materials Today Chemistry</i> , 2021, 22, 100581.	1.7	3
3180	Enhanced reversibility of vanadium oxide cathode by diminished surface precipitation in Zn(TFSI) ₂ aqueous electrolyte. <i>Electrochimica Acta</i> , 2021, 399, 139432.	2.6	16
3181	Structure and cationic distribution dependent soft magnetic properties of single-domain Mg _{1-x} Ni _x Fe ₂ O ₄ (0 ≤ x ≤ 1.0) nanocrystals. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 274, 115494.	1.7	7
3182	Effect of processing temperature on structural, optical and frequency dependent electrical responses of solid-state sintered bismuth sodium titanate. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 274, 115474.	1.7	8
3183	Structural, vibrational, electronic, elastic and thermoelectric properties of monolayer alkali halide compounds from first principles investigation. <i>Materials Today Communications</i> , 2021, 29, 102855.	0.9	4
3184	Phase stability, mechanical, thermal, electronic properties, anisotropy, lattice dynamics and APB-energies of Ti ₂ AlX intermetallics in I ₂ , B ₂ , and O phases: A first principle study. <i>Materials Today Communications</i> , 2021, 29, 102864.	0.9	2
3185	R-Ferrite-type barium cobalt stannate, BaCo ₂ Sn ₄ O ₁₁ . <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2008, 64, i71-i71.	0.2	1
3186	Structural Study of Tetragonal-Ni _{1-x} Pd _x Si/Si (001) Using Density Functional Theory (DFT). <i>Korean Journal of Materials Research</i> , 2008, 18, 482-485.	0.1	1
3187	Structural Study of Interface Layers in Tetragonal-HfO ₂ /Si using Density Functional Theory. <i>Applied Science and Convergence Technology</i> , 2009, 18, 9-14.	0.3	0
3188	Neutron Scattering Experiments at High Pressure – Experiences in ISIS. <i>Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu</i> , 2009, 19, 31-43.	0.1	2

#	ARTICLE	IF	CITATIONS
3208	Synthesis and Crystal Structure Analysis of Lithium-Ion Rechargeable Battery Anode Materials. Nihon Kessho Gakkaishi, 2013, 55, 180-187.	0.0	0
3209	The role of hydrogen bond in the phase transition of hydrous minerals. Ganseki Kobutsu Kagaku, 2013, 42, 18-24.	0.1	0
3210	Dielectric and magnetic investigations on novel P-2 type layered oxides. IOSR Journal of Applied Physics, 2014, 6, 59-69.	0.1	0
3211	Magnetism of MgO nanoparticles. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 047503.	0.2	1
3212	Development of Crystallographic Visualization Software and its Application. Nihon Kessho Gakkaishi, 2014, 56, 173-178.	0.0	0
3213	Macroscopic Electrochemical Properties Clarified by Microscopic Measurements; Present and Future. , 2014, , .		0
3214	Effects of Easy Hybrid Parallelization with CUDA for OpenMX. International Journal of Computer Applications, 2014, 98, 20-27.	0.2	0
3215	First-principles studies on the properties of Cu ₂ ZnSnS ₄ grain-boundaries due to photovoltaic effect. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 238801.	0.2	1
3216	Molecular Dynamics Simulation of the Behavior of Beryllium Diffusion in Corundum. Journal of Computer Chemistry Japan, 2015, 14, 111-116.	0.0	0
3217	Disordered Arrangements of Guest Molecules in CO Clathrate Hydrates. Hamon, 2015, 25, 22-25.	0.0	0
3219	Development of the three-dimensional visualization system for crystal, volumetric and morphology data and its application to mineralogical sciences. Ganseki Kobutsu Kagaku, 2015, 44, 52-56.	0.1	0
3220	Crystal-Local Structure Analyses for Cathode LIBs LiNi _{1-x} Co _x O ₂ (0 ≤ x ≤ 1) by Neutron Diffraction. , 2015, , .		3
3221	Na-Ion Anode Based on Na(Li,Ti)O ₂ System: Effects of Mg Addition. Journal of the Korean Ceramic Society, 2016, 53, 282-287.	1.1	0
3222	Chapter 8 Precise Structure Analysis of Inorganic Materials for Clean Energy by Maximum-Entropy Method: Neutron and Synchrotron X-Ray Powder Diffraction Studies. , 2016, , 223-244.		0
3223	Antiferro-multipole Ordered State Associated with 4f ² Configuration in Pr ₂ Zn ₂₀ . Hamon, 2017, 27, 144-147.	0.0	0
3224	Relationship between crystal morphology and twin boundary structures of quartz twinned in accordance with Japan law. Ganseki Kobutsu Kagaku, 2017, 46, 35-41.	0.1	0
3225	Structure and Electrochemical Impedance of LiNi _(x) Mn _(2-x) O ₍₄₎ . Communications in Physics, 2017, 26, 361.	0.0	0
3226	High-Pressure and High-Temperature Synthesis of Novel Hydrides Based on First-Principles Prediction. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2018, 28, 291-298.	0.1	0

#	ARTICLE	IF	CITATIONS
3227	Vapor-induced Crystallization in Alcoholic Sorption using Poly(lactic acid) Films. Journal of Applied Membrane Science & Technology, 2018, 22, .	0.3	0
3228	How Can We Control the "Element-Blocks" in Transition Metal Oxide Crystals?. , 2019, , 253-271.		0
3229	Microdisplays as a versatile tool for the optical simulation of crystal diffraction in the classroom. Journal of Applied Crystallography, 2019, 52, 457-462.	1.9	4
3230	Effects of Polymer Gel Electrolyte on Photoelectric Properties and Driving Characteristics of Prussian-Blue-Based Electrochromic Cells in Automatic Driving Circuit. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2019, 32, 33-43.	0.1	0
3231	Structural, electronic, optical properties and first-principles calculations of Sr _{1-x} Ca _x WO ₄ ceramics. Mediterranean Journal of Chemistry, 2019, 9, 199-211.	0.3	0
3232	Fine Structural Analysis Using Single Crystal Neutron Diffraction. Nihon Kessho Gakkaishi, 2019, 61, 237-242.	0.0	0
3233	From antiferromagnetism to high- T_c weak ferromagnetism manipulated by atomic rearrangement in $\text{Ba}_3\text{Mg}_2\text{O}_{10}$. Physical Review Materials, 2020, 4, .	0.9	2
3234	Direct Observation of Modulation of p - f Hybridization in Unconventional Ordered Phase of $\text{PrRu}_4\text{P}_{12}$. Journal of the Physical Society of Japan, 2020, 89, 063703.	0.7	2
3235	Possibility of ferroelectric bismuth and nitrogen co-doped barium titanate. Journal of the Ceramic Society of Japan, 2020, 128, 486-491.	0.5	3
3236	First-principles identification of ferroelectric metal-organic frameworks of $[\text{CH}_3\text{NH}_3][\text{B}(\text{HCOO})_3]$ (B = Tl, ET, Q, Rb, Cs, K, NH ₄). Over	0.784314	1
3237	Crystal structure, ionic conductivity and lithium-ion diffusion pathway in a LaCoO system. Journal of the Ceramic Society of Japan, 2020, 128, 453-456.	0.5	0
3238	Toward Zero-Strain Mixed Conductors: Anomalously Low Redox Coefficients of Chemical Expansion in Praseodymium-Oxide Perovskites. Chemistry of Materials, 0, , .	3.2	3
3239	Physical and magnetic properties of frustrated triangular-lattice antiferromagnets R_3Cu (R = Ce, Pr). Journal of Alloys and Compounds, 2022, 895, 162545.	2.8	3
3240	Polypeptoid Material as an Anchoring Material for LiS Batteries. ACS Applied Energy Materials, 2021, 4, 13070-13076.	2.5	8
3241	Low-Cost and Efficient Nickel Nitroprusside/Graphene Nanohybrid Electrocatalysts as Counter Electrodes for Dye-Sensitized Solar Cells. Materials, 2021, 14, 6563.	1.3	10
3242	M-Site Vacancy-Mediated Adsorption and Diffusion of Sodium on Ti_2CO_2 MXene. Journal of Physical Chemistry C, 2021, 125, 82-90.	1.5	10
3243	DFT Study of MAX Phase Surfaces for Electrocatalyst Support Materials in Hydrogen Fuel Cells. Materials, 2021, 14, 77.	1.3	7
3244	Impact of Sn doping on the hydrogen detection characteristics of ZnO thin films: Insights from experimental and DFT combination. Applied Surface Science, 2022, 574, 151585.	3.1	9

#	ARTICLE	IF	CITATIONS
3245	Enhancement of green upconversion luminescence and temperature sensitivity of Zr ₂ (WO ₄)(PO ₄) ₂ :Er ³⁺ ,Yb ³⁺ phosphors by co-doping Li ⁺ ions. Journal of Alloys and Compounds, 2022, 893, 162345.	2.8	8
3246	Magnon transport in the presence of antisymmetric exchange in a weak antiferromagnet. Journal of Magnetism and Magnetic Materials, 2022, 543, 168631.	1.0	1
3247	Monte Carlo calculations of Curie temperatures of Y _{1-x} Gd _x garnets. Journal of Magnetism and Magnetic Materials, 2022, 543, 168631.	1.0	1
3248	Light emission of Lu ₂ Si ₂ O ₇ pyrochlore driven by oxygen vacancy and local site engineering. Journal of Alloys and Compounds, 2022, 893, 162249.	2.8	5
3249	Developing atomistic glass models using potential-free Monte Carlo method: From simple to complex structures. Computational Materials Science, 2022, 202, 110943.	1.4	2
3250	Deciphering second harmonic generation signals. Chemical Science, 2021, 12, 15134-15142.	3.7	7
3251	Computational Methodology. Springer Theses, 2020, , 35-49.	0.0	0
3252	Compositely modulated structures of phosphor materials Sr _{1-x} Li _{2+x} Al ₂ O ₄ :Eu ²⁺ . Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 76-84.	0.5	4
3253	THEORETICAL INVESTIGATION OF DIVALENT ION INSERTION INTO TUNNEL-TYPE MANGANESE DIOXIDE POLYMORPH. OISAA Journal of Indonesia Emas, 2020, 3, 1-4.	0.0	0
3254	First principle studies of oxygen absorption on GaN(0001) surface with steps. Physica B: Condensed Matter, 2022, 627, 413528.	1.3	2
3255	Rare earth doping effect on the thermal stability of Ce _{0.35} Zr _{0.60} Mo _{0.05} O ₂ : insights from experiment and simulation. Journal of Physics: Conference Series, 2021, 2079, 012011.	0.3	0
3256	Flexibility Control of Two-Dimensional Coordination Polymers by Crystal Morphology: Water Adsorption and Thermal Expansion. Chemistry - A European Journal, 2021, 27, 18135-18140.	1.7	8
3257	Dual-Silicon-Doped Graphitic Carbon Nitride Sheet: An Efficient Metal-Free Electrocatalyst for Urea Synthesis. Journal of Physical Chemistry Letters, 2021, 12, 10837-10844.	2.1	40
3258	Photo-exfoliation of MoS ₂ quantum dots from nanosheets: an in situ transmission electron microscopy study. Nanotechnology, 2022, 33, 085601.	1.3	3
3259	Windmountainite, $\text{Fe}_3\text{Mg}_2\text{Si}_8\text{O}_{20}(\text{OH})_2(\text{H}_2\text{O})_4 \cdot 4\text{H}_2\text{O}$, a new modulated, layered Fe ³⁺ -Mg-silicate-hydrate from Wind Mountain, New Mexico: Characterization and origin, with comments on the classification of palygorskite-group minerals. Canadian Mineralogist, 2020, 58, 477-509.	0.3	3
3260	Synthesis and Characterization of Barium Titanate Nanopowders by Pechini Process. Celal Bayar Üniversitesi Fen Bilimleri Dergisi, 2020, 16, 293-300.	0.1	3
3261	Difluorochloronium(III) Fluoridometallates from Molecular Building Blocks to (Helical) Chains. European Journal of Inorganic Chemistry, 2020, 2020, 4483-4496.	1.0	2
3262	Theoretical study on stability and ion transport property with halide doping of Na ₃ SbS ₄ electrolyte for all-solid-state batteries. Journal of Materials Chemistry A, 2022, 10, 2235-2248.	5.2	17

#	ARTICLE	IF	CITATIONS
3263	Structural properties of $\text{Co}_x\text{Cu}_{1-x}\text{Fe}_2\text{O}_4$ solid solution ^{**} . <i>Journal of the Mechanical Behavior of Materials</i> , 2021, 30, 220-227.	0.7	7
3264	Asymmetric janus functionalities induced changes in structural, electronic, optical characteristics of MXenes $\text{Ta}_4\text{C}_3\text{Tx}$. <i>Solid State Communications</i> , 2022, 341, 114585.	0.9	3
3265	Atomic insights into the ordered solid solutions of Ni and Au in $\hat{\text{I}}\text{-Cu}_6\text{Sn}_5$. <i>Acta Materialia</i> , 2022, 224, 117513.	3.8	3
3266	D ⁺ based pyrido-pyrazino[2,3-b]indole amines as blue-red fluorescent dyes: Photophysical, aggregation-induced emission, electrochemical and theoretical studies. <i>Journal of Luminescence</i> , 2022, 242, 118568.	1.5	16
3267	Molecular dynamics studies on separation of CO_2/CH_4 by the ionic liquids encapsulated ZIF-8. <i>Journal of Membrane Science</i> , 2022, 644, 120117.	4.1	6
3268	Thickness and composition of native oxides and near-surface regions of Ni superalloys. <i>Journal of Alloys and Compounds</i> , 2022, 895, 162657.	2.8	33
3269	Fabrication and characterization of high entropy pyrochlore ceramics. <i>Boletin De La Sociedad Espanola De Ceramica Y Vidrio</i> , 2023, 62, 66-76.	0.9	9
3270	Reconstruction and electronic properties of $\hat{\text{I}}^2\text{-Li}_3\text{PS}_4 \text{Li}_2\text{S}$ interface. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 105305.	1.3	6
3271	Antiperovskite Superconductor LaPd_3P with Noncentrosymmetric Cubic Structure. <i>Inorganic Chemistry</i> , 2021, 60, 18017-18023.	1.9	7
3272	Predicting synthesizability of crystalline materials via deep learning. <i>Communications Materials</i> , 2021, 2, .	2.9	18
3273	P 4 S 10 Modification for Lithium Metal Anode Surface. <i>Physica Status Solidi (B): Basic Research</i> , 0, , 2100455.	0.7	1
3274	Structure and Surface Passivation of Ultrathin Cesium Lead Halide Nanoplatelets Revealed by Multilayer Diffraction. <i>ACS Nano</i> , 2021, 15, 20341-20352.	7.3	17
3275	RbCeX_2 Crystal (X = S, Se, Te): Pressure-Induced Spin-Selective Gapless Transition and Response Properties. <i>Journal of Alloys and Compounds</i> , 2022, 898, 162760.	2.8	3
3276	Bipyridine carboxylic acid as a high-performance anode material for lithium- and sodium-ion batteries. <i>Electrochimica Acta</i> , 2022, 405, 139628.	2.6	8
3277	Magnetic properties of 3d, 4d, and 5d transition-metal atomic monolayers in Fe/TM/Fe sandwiches: Systematic first-principles study. <i>Journal of Magnetism and Magnetic Materials</i> , 2022, 546, 168828.	1.0	5
3278	Li migration, nucleation and growth behavior regulated by a lithiophilic cobalt phosphide-doped carbon nanofibers derived ion/electron conductive framework. <i>Energy Storage Materials</i> , 2022, 45, 1109-1119.	9.5	30
3279	<i>r</i> mc-discord: reverse Monte Carlo refinement of diffuse scattering and correlated disorder from single crystals. <i>Journal of Applied Crystallography</i> , 2021, 54, 1867-1885.	1.9	6
3280	Promoting Electrochemical Performance of $\text{Ti}_3\text{C}_2\text{O}_2$ MXene-Based Electrodes of Alkali-Ion Batteries via S Doping: Theoretical Insight. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 57306-57316.	4.0	16

#	ARTICLE	IF	CITATIONS
3281	Green synthesis, structure feature and energy transfer of yellow-emitting (Y,Gd) ₂ O ₂ SO ₄ :Dy phosphors. <i>Luminescence</i> , 2022, 37, 199-207.	1.5	4
3282	Co-existence of short- and long-range magnetic order in LaCo ₂ P ₂ . <i>Physica Scripta</i> , 0, , .	1.2	2
3283	Crystal structure of the high- <i>P</i> polymorph of Ca ₂ B ₆ O ₆ (OH) ₁₀ ·2(H ₂ O) (meyerhofferite). <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 940-945.	0.5	4
3284	Superconductivity in In-doped AgSnBiTe ₃ with possible band inversion. <i>Scientific Reports</i> , 2021, 11, 22885.	1.6	4
3285	Direct observation of one-dimensional disordered diffusion channel in a chain-like thermoelectric with ultralow thermal conductivity. <i>Nature Communications</i> , 2021, 12, 6709.	5.8	21
3286	Quasiparticle electronic structure of phthalocyanine:TMD interfaces from first-principles <i>GW</i> . <i>Journal of Chemical Physics</i> , 2021, 155, 214702.	1.2	9
3287	Tailoring of structural, optical and electrical properties of anatase TiO ₂ via doping of cobalt and nitrogen ions. <i>Journal of Materials Science and Technology</i> , 2022, 111, 287-297.	5.6	23
3288	Complex correlations between microstructure and magnetic behavior in SrFe ₁₂ O ₁₉ hexaferrite nanoparticles. <i>Scientific Reports</i> , 2021, 11, 23307.	1.6	11
3289	Intrinsic Nature of Spontaneous Magnetic Fields in Superconductors with Time-Reversal Symmetry Breaking. <i>Physical Review Letters</i> , 2021, 127, 237002.	2.9	13
3290	Detailed study on optical properties of Li ₂ B ₄ O ₇ for down-conversion to millimeter waves. , 2021, , .		0
3291	Effect of La vacancies on the oxide-ion conduction in lanthanum silicate apatites. <i>Solid State Ionics</i> , 2021, 373, 115793.	1.3	2
3292	A study on the stability of gold copper bimetallic clusters on the CeO ₂ (110) surface. <i>Catalysis Communications</i> , 2022, 162, 106376.	1.6	8
3293	Mn-Dopant Induced Octahedral Configuration Strongly Stabilizes Ni ₁₂ P ₅ Nanowires for Battery-Supercapacitor Hybrid Devices. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3294	FEATURES OF SIMULATION OF CHARACTERISTICS OF THERMOMETRIC MATERIAL Lu _{1-x} Zr _x NiSb. <i>Measuring Equipment and Metrology</i> , 2021, 82, 12-17.	0.1	1
3295	First-principles search of hot superconductivity in La-X-H ternary hydrides. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	25
3296	Exploration of a large-scale reconstructed structure on GaN(0001) surface by Bayesian optimization. <i>Applied Physics Letters</i> , 2022, 120, 021602.	1.5	7
3297	Temperature dependent structural, dielectric, Raman, piezoresponse and photoluminescence investigations in sol-gel derived BCZT ceramics. <i>Materials Chemistry and Physics</i> , 2022, 277, 125526.	2.0	5
3298	Thermal enhancement of 2H _{11/2} → ⁴ I _{15/2} up-conversion luminescence of BaLu ₆ (Si ₂ O ₇) ₂ (Si ₃ O ₁₀):Er ³⁺ /Yb ³⁺ phosphors. <i>Optik</i> , 2022, 252, 168544.	1.4	1

#	ARTICLE	IF	CITATIONS
3299	Recommendation of interstitial hydrogen positions in metal oxides. Computational Materials Science, 2022, 203, 111068.	1.4	2
3300	Temperature dependent magnetization in Co@Fe Nanoparticles. Physica B: Condensed Matter, 2022, 627, 413488.	1.3	7
3301	Tailoring Bi ₂ MoO ₆ by Eu ³⁺ incorporation for enhanced photoluminescence emissions. Journal of Luminescence, 2022, 243, 118675.	1.5	9
3302	Cs ₂ Bi ₂ Sr(P ₂ O ₇)(PO ₄) ₂ :Er ³⁺ /Yb ³⁺ phosphors for outstanding thermal enhancement of up-conversion under 980 and 1550Ånm laser excitations in the 303 to 723ÅK range. Chemical Engineering Journal Advances, 2022, 10, 100242.	2.4	4
3303	Computational design of materials for metal-ion batteries. , 2023, , 404-429.		4
3304	A Key Role of Soft and Refractory Coke in the Deactivation of Al_2O_3 Catalysts During Low-Temperature Methyl Oleate Epoxidation. SSRN Electronic Journal, 0, , .	0.4	0
3305	Magnetic phase transitions in the LiNi _{0.9} M _{0.1} PO ₄ (M=ÅMn, Co) single crystals. Physica Scripta, 2022, 97, 025707.	1.2	1
3306	Evaluation of the Structure–Micromorphology Relationship of Co _{10%} –Al _x Co-doped Zinc Oxide Nanostructured Thin Films Deposited by Pulsed Laser Using XRD and AFM. Arabian Journal for Science and Engineering, 2022, 47, 7717-7728.	1.7	6
3307	Differentiating Defects and Their Influence on Hematite Photoanodes Using X-ray Absorption Spectroscopy and Raman Microscopy. ACS Applied Materials & Interfaces, 2022, 14, 6615-6624.	4.0	11
3308	Dynamics of complex impedance, dielectric and electric modulus for NiCuZn ferrites with theoretical justification. International Nano Letters, 2022, 12, 179-190.	2.3	4
3309	Effect of Ca ²⁺ doping on the electronic charge density and magnetic properties of ZnFe ₂ O ₄ spinel ferrites. Journal of Materials Science: Materials in Electronics, 2022, 33, 4116-4131.	1.1	9
3310	Electrochromic Behavior Originating from the W ⁶⁺ /W ⁵⁺ Redox in Aurivillius-type Tungsten-Based Layered Perovskites. Inorganic Chemistry, 2022, 61, 2509-2516.	1.9	10
3311	Elastic properties of Janus transition metal dichalcogenide nanotubes from first principles. European Physical Journal B, 2022, 95, 1.	0.6	5
3312	A metallic Cu ₂ N monolayer with planar tetracoordinated nitrogen as a promising catalyst for CO ₂ electroreduction. Journal of Materials Chemistry A, 2022, 10, 1560-1568.	5.2	13
3313	van der Waals graphene/MoS ₂ heterostructures: tuning the electronic properties and Schottky barrier by applying a biaxial strain. Materials Advances, 2022, 3, 624-631.	2.6	18
3314	Oxidation or cation re-arrangement? Distinct behavior of riebeckite at high temperature. American Mineralogist, 2022, , .	0.9	0
3315	Phosphors of Rb ₃ La ³⁺ with K ₃ NdSi ₂ O ₇ -type structure. Journal of the Ceramic Society of Japan, 2022, 130, 44-48.	0.5	0
3316	Investigation of electronic structure, morphological features, optical, colorimetric, and supercapacitor electrode properties of CoWO ₄ crystals. Materials Science for Energy Technologies, 2022, 5, 125-144.	1.0	8

#	ARTICLE	IF	CITATIONS
3317	Polaron Induced Conductance Switching in Conjugated Oligophenylene: A First-Principles Analysis. <i>Journal of Physical Chemistry A</i> , 2022, 126, 318-324.	1.1	1
3318	Mechanism investigation of the enhanced oxygen storage performance of $\text{YBaCo}_4\text{O}_{7+\delta}$ synthesized by a glycine-complex decomposition method. <i>Chemical Communications</i> , 2022, 58, 2822-2825.	2.2	0
3319	Tuning the Interaction between Ruthenium Single Atoms and the Second Coordination Sphere for Efficient Nitrogen Photofixation. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	22
3320	Correlating Broadband Photoluminescence with Structural Dynamics in Layered Hybrid Halide Perovskites. <i>Journal of the American Chemical Society</i> , 2022, 144, 1313-1322.	6.6	37
3321	Density Functional Theory Studies on Li Metal Electrode/Garnet-Type $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolyte Interfaces for Application in All-Solid-State Batteries. <i>Physica Status Solidi (B): Basic Research</i> , 2022, 259, .	0.7	4
3322	Pressure driven structural phase transition in EuTaO_4 : experimental and first principles investigations. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 135401.	0.7	3
3323	Borazatruxenes as precursors for hybrid C-BN 2D molecular networks. <i>Nanoscale</i> , 2022, 14, 1929-1943.	2.8	2
3324	Deformation and Failure Mechanisms of Thermoelectric Type-I Clathrate $\text{Ba}_8\text{Au}_6\text{Ge}_{40}$. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 4326-4334.	4.0	1
3325	Theoretical Prediction of Mixed-Valence Layered Halide Perovskites $\text{Cs}_4\text{M(IV)M(II)}_2\text{X}_{12}$ (M = Ge, Sn; X = Cl, Br). <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1077-1084.	2.1	3
3326	Surface functionalization of few-layer graphene on $\text{SiC}(001)$ by Neutral Red dye. <i>Applied Surface Science</i> , 2022, 585, 152542.	3.1	4
3327	All-Atom Nonadiabatic Dynamics Simulation of Hybrid Graphene Nanoribbons Based on Wannier Analysis and Machine Learning. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 22929-22940.	4.0	10
3328	Study of structural correlations with temperature dependent dielectric response and ferroelectric behavior for (Sr, Mn) co-doped BaTiO_3 . <i>Journal of Materials Science: Materials in Electronics</i> , 2022, 33, 6329-6353.	1.1	10
3329	Reversible Charge/Discharge Reaction of a Ternary Metal Fluoride, Pb_2CuF_6 : A Highly Conductive Cathode Material for Fluoride-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2022, 5, 1002-1009.	2.5	10
3330	High-pressure behaviour and atomic-scale deformation mechanisms in inyoite, $\text{CaB}_3\text{O}_3(\text{OH})_5 \cdot 4\text{H}_2\text{O}$. <i>Physics and Chemistry of Minerals</i> , 2022, 49, 1.	0.3	5
3331	Operando XRD studies on Bi_2MoO_6 as anode material for Na-ion batteries. <i>Nanotechnology</i> , 2022, 33, 185402.	1.3	9
3332	High-pressure phases of a Mn-N system. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1830-1839.	1.3	5
3333	Heterostructural MoS_2/NiS nanoflowers via precise interface modification for enhancing electrocatalytic hydrogen evolution. <i>New Journal of Chemistry</i> , 2022, 46, 5505-5514.	1.4	8
3334	Vibrational Property of $\hat{I}\pm$ -Borophene Determined by Tip-Enhanced Raman Spectroscopy. <i>Molecules</i> , 2022, 27, 834.	1.7	4

#	ARTICLE	IF	CITATIONS
3335	Structural, electronic and magnetic properties of the Half-Heusler alloy CrZSi (Z = Sc, Ti). Journal of Crystal Growth, 2022, 583, 126556.	0.7	12
3336	Hydrothermal synthesis and crystal structure of a novel double-perovskite-type bismuth oxide with 3d ⁰ ordering at the B-site. New Journal of Chemistry, 2022, 46, 3595-3601.	1.4	5
3337	Magnetic properties of Gd ₃ CuSb ₇ . Journal of Applied Physics, 2022, 123, 154101.	1.0	1
3338	Microstructural characterization and phase analysis of new pyrochlore-type mixed metal oxides RESmTi ₂ O ₇ (RE = Gd, Er) by X-ray powder diffraction using Rietveld refinement method and spectroscopic studies. Ceramics International, 2022, 48, 13651-13658.	2.3	6
3339	Hydrothermal synthesis and crystal structure of a new rubidium sodium niobium fluoride, RbNaNb ₇ F ₂₁ . Journal of the Ceramic Society of Japan, 2022, 130, 232-235.	0.5	1
3340	The joint effect of spin-orbit coupling and atomistic disorder on bandgap evolution in inorganic CsSn _{1-x} Pbx ₃ mixed perovskite. Journal of Applied Physics, 2022, 131, 055107.	1.1	1
3341	A new salt-inclusion compound, Ag ₄ Br @ [B ₇ O ₁₂], with a novel type of the porous double-layered borate anion and strong anharmonicity of the ϵ -sublattice. Solid State Sciences, 2022, 125, 106831.	1.5	4
3342	Defects on Li ₂ S@graphene cathode improves the performance of lithium-sulfur battery, A theoretical study. Acta Materialia, 2022, 226, 117632.	3.8	10
3343	Study of new lead-free double perovskites halides Tl ₂ TiX ₆ (X = Cl, Br, I) for solar cells and renewable energy devices. Journal of Solid State Chemistry, 2022, 308, 122887.	1.4	31
3344	Interfacial covalent bonding enables transition metal phosphide superior lithium storage performance. Applied Surface Science, 2022, 582, 152404.	3.1	22
3345	First-principles insight into the interfacial properties of epitaxial Bi ₂ O ₂ X (X = S, Se, Te) on SrTiO ₃ substrates. Journal of Physics and Chemistry of Solids, 2022, 163, 110601.	1.9	5
3346	Highly CO-Selective Mixed-Matrix membranes incorporated with Ag Nanoparticle-Impregnated MIL-101 Metal-Organic frameworks. Chemical Engineering Journal, 2022, 435, 134803.	6.6	8
3347	Temperature-dependent magnetodielectric, magnetoimpedance, and magnetic field controlled dielectric relaxation response in KBiFe ₂ O ₅ . Journal of Magnetism and Magnetic Materials, 2022, 549, 169047.	1.0	10
3348	$\hat{\Gamma}_{\pm}$ Ag ₂ WO ₄ under microwave, electron beam and femtosecond laser irradiations: Unveiling the relationship between morphology and photoluminescence emissions. Journal of Alloys and Compounds, 2022, 903, 163840.	2.8	3
3349	Temperature dependency on Ce-doped CuO nanoparticles: a comparative study via XRD line broadening analysis. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	13
3350	Energies and structures of Cu/Nb and Cu/W interfaces from density functional theory and semi-empirical calculations. Materialia, 2022, 21, 101362.	1.3	13
3351	Models of Ni- and Co-ion occupation in LiNi _{0.5} Co _{0.5} PO ₄ orthophosphate and its magnetic structure. Journal of Physics Condensed Matter, 2022, , .	0.7	0
3352	Improved oxide-ion conductivity by substitution of Sr for Bi in Dion-Jacobson phase CsBi ₂ Ti ₂ NbO ₁₀ . Ceramics International, 2022, 48, 16522-16528.	2.3	3

#	ARTICLE	IF	CITATIONS
3353	Thermoelectric performance in the binary semiconductor compound $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{A} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{K, Rb} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle =$ K, Rb) with host-guest structure. <i>Physical Review B</i> , 2022, 105, .	1.1	25
3354	Ab initio comparative study of B2 $\hat{\epsilon}$ "MnX intermetallics with X $\hat{\epsilon}$ % $\hat{\epsilon}$ %V, Nb, Ta. <i>European Physical Journal B</i> , 2022, 95, 1.	0.6	1
3355	Role of lithium intercalation in fluorine-doped tin oxide thin films: Ab-initio calculations and experiment. <i>Journal of Chemical Physics</i> , 2022, 156, 094701.	1.2	2
3356	Experimental and DFT investigations of the performance of ZrO ₂ catalysts modified with Ce, La, Y, Mg, and Ba oxides during methyl stearate ketonization. <i>Applied Surface Science</i> , 2022, 585, 152627.	3.1	5
3357	Study of different structures derives of $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \text{ display="inline" id="d1e1000" altimg="si2.svg"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \hat{I}^2 \langle \text{mml:mi} \rangle \langle \text{mml:mo} \text{ linebreak="goodbreak" linebreakstyle="after"} \rangle \hat{\sim} \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \text{C} \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{u} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle$ by means of ab-initio calculations and Quasi-Harmonic Approximation. <i>Computational Condensed Matter</i> , 2022, 31, e00652.	0.9	2
3358	High- <i>T_c</i> Superconducting Hydrides Formed by LaH ₂₄ and YH ₂₄ Cage Structures as Basic Blocks. <i>Chemistry of Materials</i> , 2021, 33, 9501-9507.	3.2	16
3359	Studies on Structural and Thermodynamic Properties of Charge Coupled Substituted NaxCa _{10-2x} (PO ₄) ₆ F ₂ Solid Solutions (X=0.5 to 2.0). <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3360	Blue-red emitting materials based on a pyrido[2,3- <i>b</i>]pyrazine backbone: design and tuning of the photophysical, aggregation-induced emission, electrochemical and theoretical properties. <i>RSC Advances</i> , 2022, 12, 6888-6905.	1.7	9
3361	Atomistic insight into the dopant impacts at the garnet Li ₇ La ₃ Zr ₂ O ₁₂ solid electrolyte grain boundaries. <i>Journal of Materials Chemistry A</i> , 2022, 10, 10083-10091.	5.2	13
3362	Structural and thermal properties of ultralow thermal conductivity Ba ₃ Cu ₂ Sn ₃ Se ₁₀ . <i>Dalton Transactions</i> , 2022, 51, 6220-6225.	1.6	3
3363	Lattice Instability and Raman Spectra of Bao Under High Pressure: A First Principles Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3364	Mapping of the Degradation Processes at Bifunctional O ₂ Gas Diffusion Electrode for Aqueous Alkaline Metal-Air Batteries. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3365	More complex than originally thought: revisiting the origins of the relaxation processes in dimethylammonium zinc formate. <i>Journal of Materials Chemistry C</i> , 2022, 10, 6866-6877.	2.7	5
3366	A theoretical investigation of the hydrolysis of uranium hexafluoride: the initiation mechanism and vibrational spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9634-9647.	1.3	4
3367	Structural Diversity and Unusual Valence States in Compressed Na-Hg System. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3368	Influence of Zn ²⁺ Doping on CaFe ₂ O ₄ Spinel Ferrites: An Analysis of Experimental Charge Density and Magnetism. <i>Journal of Superconductivity and Novel Magnetism</i> , 2022, 35, 1281-1298.	0.8	4
3369	Intrinsic Defects, Diffusion and Dopants in AVSi ₂ O ₆ (A = Li and Na) Electrode Materials. <i>Batteries</i> , 2022, 8, 20.	2.1	1
3370	Engineering Lattice Disorder on a Photocatalyst: Photochromic BiOBr Nanosheets Enhance Activation of Aromatic C-H Bonds via Water Oxidation. <i>Journal of the American Chemical Society</i> , 2022, 144, 3386-3397.	6.6	96

#	ARTICLE	IF	CITATIONS
3371	High-Temperature Thermoelectric Monolayer Bi ₂ TeSe ₂ with High Power Factor and Ultralow Thermal Conductivity. ACS Applied Energy Materials, 2022, 5, 2564-2572.	2.5	35
3372	Teaching basic crystallography and diffraction using open access structure visualization software. MRS Advances, 2022, 7, 482-487.	0.5	6
3373	Observation of a Novel Lattice Instability in Ultrafast Photoexcited SnSe. Physical Review X, 2022, 12, .	2.8	10
3374	Quantifying fish otolith mineralogy for trace-element chemistry studies. Scientific Reports, 2022, 12, 2727.	1.6	7
3375	Correlating Symmetries of Low-Frequency Vibrations and Self-Trapped Excitons in Layered Perovskites for Light Emission with Different Colors. Small, 2022, , 2106759.	5.2	10
3376	Dissolution of Portlandite in Pure Water: Part 2 Atomistic Kinetic Monte Carlo (KMC) Approach. Materials, 2022, 15, 1442.	1.3	19
3377	Pressure-Induced Phase Transition and Band Gap Decrease in Semiconducting $\text{I}^2\text{-Cu}_2\text{V}_2\text{O}_7$. Inorganic Chemistry, 2022, 61, 3697-3707.	1.9	7
3378	Understanding Separation Mechanisms of Monoatomic Gases, Such as Kr and Xe, via DD3R Zeolite Membrane Using Molecular Dynamics. Thermo, 2022, 2, 56-73.	0.6	1
3379	Manipulation of spin orientation via ferroelectric switching in Fe-doped Bi_2WO_6 from first principles. Physical Review B, 2022, 105, .	1.1	4
3380	Structural refinement and antimicrobial activity of aluminum oxide nanoparticles. Journal of the Ceramic Society of Japan, 2022, 130, 257-263.	0.5	4
3381	Processing, phase evolution and electrical properties of lead free KNN-BF-CuO eco-piezoceramic from mechanochemically activated precursors. Open Ceramics, 2022, 9, 100247.	1.0	1
3382	Compressibility of structural modulation waves in the chain compounds BaCo_2O_7 ($X = \text{As}, \text{P}$): a powder study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 162-171.	0.5	0
3383	Fast-Charging Halide-Based All-Solid-State Batteries by Manipulation of Current Collector Interface. Advanced Functional Materials, 2022, 32, .	7.8	20
3384	Improvement of critical current density of $\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ by increase in configurational entropy of mixing. Royal Society Open Science, 2022, 9, 211874.	1.1	6
3385	Local structure and electron density distribution analysis of tin(II) sulfide using pair distribution function and maximum entropy method. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2022, 77, 689-700.	0.7	0
3386	Pressure-induced transitions in RCo_5 ($R = \text{Y}, \text{La}$) studied by x-ray emission spectroscopy, x-ray diffraction and density functional theory. Journal of Physics Condensed Matter, 2022, , .	0.7	0
3387	π -Hole bonding in a new co-crystal hydrate of gallic acid and pyrazine: static and dynamic charge density analysis. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 231-246.	0.5	4
3388	Insight into the underlying competitive mechanism for the shift of the charge neutrality point in a trilayer-graphene field-effect transistor. EScience, 2022, 2, 319-328.	25.0	14

#	ARTICLE	IF	CITATIONS
3389	Detailed Structural Features of the Perovskite-Related Halide RbPbI_3 for Solar Cell Applications. <i>Inorganic Chemistry</i> , 2022, 61, 5502-5511.	1.9	7
3390	Development of 2NN MEAM potential for Fe-Al and atomistic investigation of surface and interface properties of the inhibition layer in galvanized Fe. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2022, 30, 045001.	0.8	2
3391	A comparative study on the stability of the furfural molecule on the low index Ni, Pd and Pt surfaces. <i>Royal Society Open Science</i> , 2022, 9, 211516.	1.1	4
3392	Chemistry, Structure, and Function of Lone Pairs in Extended Solids. <i>Accounts of Chemical Research</i> , 2022, 55, 1004-1014.	7.6	32
3393	First-Principles Analysis of the Oxide-Ion Conduction Mechanism in Si-Deficient Lanthanum Silicate Apatite. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5805-5812.	1.5	3
3394	Pressure-induced emission enhancement and bandgap narrowing: Experimental investigations and first-principles theoretical simulations on the model halide perovskite $\text{Cs}_3\text{Bi}_2\text{I}_8$. <i>Physical Review B</i> , 2022, 105, .	1.1	8
3395	Structural phase transitions and magnetic superexchange in $\text{Mg}_2\text{Ag}_2\text{IF}_3$ perovskites at high pressure. <i>Chemistry - A European Journal</i> , 2022, .	1.7	1
3396	Aqueous spray-drying synthesis of alluaudite $\text{Na}_{2+2x}\text{Fe}_2\text{x}(\text{SO}_4)_3$ sodium insertion material: studies of electrochemical activity, thermodynamic stability, and humidity-induced phase transition. <i>Journal of Solid State Electrochemistry</i> , 2022, 26, 1941-1950.	1.2	5
3397	Strain engineering of Janus transition metal dichalcogenide nanotubes: an ab initio study. <i>European Physical Journal B</i> , 2022, 95, 1.	0.6	4
3398	Multiscale nucleation growth model of yttrium oxide during the deoxidation of Fe-O melt. <i>Journal of Materials Science</i> , 2022, 57, 6988-7000.	1.7	3
3399	Tuning electronic properties and ferromagnetism of CrI_3 monolayers with doped transition-metal atoms. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 265303.	1.3	2
3400	Magnetoelastic coupling anisotropy in the Kitaev material RuCl_3 . <i>Physical Review B</i> , 2022, 105, .		
3401	Polymer Structure Predictor (PSP): A Python Toolkit for Predicting Atomic-Level Structural Models for a Range of Polymer Geometries. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2737-2748.	2.3	7
3402	Detection of cracked teeth using a mechanoluminescence phosphor with a stretchable photodetector array. <i>NPG Asia Materials</i> , 2022, 14, .	3.8	11
3403	First-principles based study of magnetic states and high-pressure enthalpy landscape of manganese sulfide polymorphs. <i>Journal of Applied Physics</i> , 2022, 131, 115904.	1.1	1
3404	Room Temperature Magnetism and Experimental Electron Density Analysis of Co^{2+} Doped ZnFe_2O_4 Spinel Nanoferrites. <i>Journal of Electronic Materials</i> , 0, , 1.	1.0	5
3405	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors. <i>Research</i> , 2022, 2022, 9857631.	2.8	4
3406	Electronic structure of YbFe_4Al_8 antiferromagnet: A combined X-ray photoelectron spectroscopy and first-principles study. <i>Journal of Alloys and Compounds</i> , 2022, 910, 164478.	2.8	1

#	ARTICLE	IF	CITATIONS
3407	First principle calculations on pristine and Mn-doped iron fluorophosphates as sodium-ion battery cathode materials. Computational Materials Science, 2022, 206, 111292.	1.4	7
3408	Recent advances in the application of machine-learning algorithms to predict adsorption energies. Trends in Chemistry, 2022, 4, 347-360.	4.4	4
3409	Oxygen Vacancy Formation and Migration within the Antiphase Boundaries in Lanthanum Scandate-Based Oxides: Computational Study. Materials, 2022, 15, 2695.	1.3	0
3410	Identification of potential metal oxides for NO ₂ capture: A density functional theory study. Journal of the American Ceramic Society, 2022, 105, 5299-5308.	1.9	3
3411	Synthesis and Characterization of High-Entropy-Alloy-Type Layered Telluride MBi ₂ Te ₄ (M = Ag, In, Sn, Pb). <i>Tj ETQq0,0,0 rgBT /Overlock 1</i>	1.3	1
3412	Giant Tunneling Electroresistance Induced by Interfacial Doping in $\text{Ba}_x\text{Bi}_{1-x}\text{O}_3$ Ferroelectric Tunnel Junctions. Physical Review Applied, 2022, 17, .		
3413	Enhanced reversible hydrogen storage performance of light metal-decorated boron-doped siligene: A DFT study. International Journal of Hydrogen Energy, 2022, 47, 41310-41319.	3.8	26
3414	Accurate and efficient approximate quasiparticle DFT $\frac{1}{2}$ band structure calculations of transition metal oxide perovskites. Physica Status Solidi (B): Basic Research, 0, , .	0.7	0
3415	Fully Chelating N ₃ O ₂ -Pentadentate Planar Ligands Designed for the Strongest and Selective Capture of Uranium from Seawater. Inorganic Chemistry, 2022, 61, 6175-6181.	1.9	3
3416	Correlation between <i>d</i> -orbital bandwidth and local coordination environment in RE ₂ SiO ₅ compounds with implications in minimizing the coefficient of thermal expansion anisotropy (RE = Sc, Y, La). AIP Advances, 2022, 12, 045012.	0.6	1
3417	Synergistic interaction of Nb atoms anchored on g-C ₃ N ₄ and H ⁺ promoting high-efficiency nitrogen reduction reaction. Chinese Journal of Catalysis, 2022, 43, 1139-1147.	6.9	14
3418	Exploring a high-carrier-mobility black phosphorus/MoSe ₂ heterostructure for high-efficiency thin film solar cells. Solar Energy, 2022, 236, 576-585.	2.9	13
3419	Enhanced electrochemical properties of W-doped Na ₃ V ₂ (PO ₄) ₂ F ₃ @C as cathode material in sodium ion batteries. Electrochimica Acta, 2022, 415, 140256.	2.6	12
3420	Determination of thermodynamic growth conditions for a high-efficiency Cu Si_{10}		

#	ARTICLE	IF	CITATIONS
3425	A key role of soft and refractory coke in the deactivation of $\gamma\text{-Al}_2\text{O}_3$ catalysts during low-temperature methyl oleate epoxidation: An experiment and DFT study. <i>Fuel</i> , 2022, 321, 124064.	3.4	2
3426	$\text{Na}_3\text{V}_2\text{-xFex(PO}_4)_2\text{O}_2\text{F}$: An advanced cathode material with ultra-high stability for superior sodium storage. <i>Chemical Engineering Journal</i> , 2022, 441, 136132.	6.6	11
3427	Stability and electronic structure of magnesium hydride and magnesium deuteride under high pressure. <i>Journal of Physics: Conference Series</i> , 2021, 2145, 012026.	0.3	1
3428	Operando XAS of a Bifunctional Gas Diffusion Electrode for Zn-Air Batteries under Realistic Application Conditions. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 11672.	1.3	6
3429	Anomalous suppressed thermal conductivity in CuInTe_2 under pressure. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	11
3430	Novel polymorphs and polytypes of lithium chloride from structure predictions based on charge equilibration via neural network technique. <i>Physical Review Materials</i> , 2021, 5, .	0.9	2
3431	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in $\text{Cu}_2\text{ZnSnS}_4$ Photoabsorbers. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 61365-61373.	4.0	11
3432	Transport spin polarization of noncollinear antiferromagnetic antiperovskites. <i>Physical Review Materials</i> , 2021, 5, .	0.9	10
3433	Carrier tuning of Stoner ferromagnetism in ThCr_2Mn_6 -structure cobalt arsenides. <i>Physical Review B</i> , 2021, 104, .	1.1	1
3434	First-Principles Study of Optical Absorption Energies, Ligand Field and Spin-Hamiltonian Parameters of Cr^{3+} Ions in Emeralds. <i>Inorganic Chemistry</i> , 2022, 61, 178-192.	1.9	10
3435	Kinetically Controlled Reduction of V^{5+} -Vanadyl(V) Orthophosphate: Synthesis and Characterization of New Metastable Polymorphs of Vanadium(III) Phosphate. <i>Inorganic Chemistry</i> , 2022, 61, 507-519.	1.9	0
3436	Low-temperature domain-wall freezing and nonequilibrium dynamics in the transverse-field Ising model material CoNb_2O_6 . <i>Physical Review B</i> , 2021, 104, .	1.1	0
3437	Could network structures generated with simple rules imposed on a cubic lattice reproduce the structural descriptors of globular proteins?. <i>Journal of Complex Networks</i> , 2021, 10, .	1.1	0
3438	Posttreatment Effects on the Crystal Structure and Superconductivity of Ca-Free Double-Layered Cuprate $\text{Sr}_2\text{SrCu}_2\text{O}_{4+y}\text{F}_2$. <i>Chemistry of Materials</i> , 2021, 33, 9690-9697.	3.2	1
3439	Elastic Properties and Deformation Mechanisms in the van der Waals Single-Crystalline Indium Selenide. <i>Physica Status Solidi - Rapid Research Letters</i> , 2022, 16, 2100418.	1.2	1
3440	Revealing Atomic-Scale Ionic Stability and Transport around Grain Boundaries of Garnet $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolyte. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	25
3442	Si doped T-graphene: a 2D lattice as an anode electrode in Na ion secondary batteries. <i>New Journal of Chemistry</i> , 2022, 46, 9718-9726.	1.4	10
3443	Effect of aluminum addition on the structure and electronic properties of boron nitride. <i>Journal of Solid State Chemistry</i> , 2022, 311, 123153.	1.4	3

#	ARTICLE	IF	CITATIONS
3444	Estimation of the Gr ^{1/4} neisen Parameter of High-Entropy Alloy-Type Functional Materials: The Cases of REO _{0.7} FO _{0.3} BiS ₂ and MTe. Condensed Matter, 2022, 7, 34.	0.8	0
3445	Crystal Structure of Tengchongite with a Revised Chemical Formula Ca(UO ₂) ₆ (MoO ₄ OH)2O ₂ (OH)4·9H ₂ O. Canadian Mineralogist, 2022, , .	0.3	1
3446	Topological superconductivity in Rashba spin-orbital coupling suppressed monolayer \hat{I}^2 -Bi ₂ Pd. Materials Today Physics, 2022, 24, 100674.	2.9	6
3447	Polymorphism and sodium-ion conductivity of NaTa ₂ PO ₈ synthesized via the Li ⁺ /Na ⁺ ion-exchange reaction of LiTa ₂ PO ₈ . Ceramics International, 2022, 48, 20712-20720.	2.3	1
3448	High-Rate Lithium Cycling and Structure Evolution in Mo ₄ O ₁₁ . Chemistry of Materials, 2022, 34, 4122-4133.	3.2	13
3449	YVO ₄ :RE (RE = Eu, Tm, and Yb/Er) nanoparticles synthesized by the microwave-assisted hydrothermal method for photoluminescence application. Ectetica Quimica, 2022, 47, 39-49.	0.2	2
3450	Insights into the activity of single-atom Fe-N-C catalysts for oxygen reduction reaction. Nature Communications, 2022, 13, 2075.	5.8	197
3451	Periodicity of Superatomic Hybrid Orbitals in Substituted Superatoms and Superatomic-like X@Ga ₁₂ (X) Tj ETQq1 1.0,784314 rgBT /Qv	1.0	1
3452	Investigation of structural, magnetic and electronic properties of CoMnSb superstructure: A DFT study. Computational Materials Science, 2022, 210, 111441.	1.4	3
3455	In Situ Orthorhombic to Amorphous Phase Transition of Nb ₂ O ₅ and Its Temperature Effect on Pseudocapacitive Behavior. ACS Applied Materials & Interfaces, 2022, 14, 19426-19436.	4.0	13
3456	Stabilizing superconductivity of ternary metal pentahydride CaCH_5 via electronic topological transitions under high pressure from first principles evolutionary algorithm. Scientific Reports, 2022, 12, 6700.	1.6	3
3457	Why Local and Non-local Terms are Essential for Second Harmonic Generation Simulation?. Physical Chemistry Chemical Physics, 2022, , .	1.3	3
3458	Pressure-driven thermoelectric properties of defect chalcopyrite structured ZnGa ₂ Te ₄ : <i>ab initio</i> study. RSC Advances, 2022, 12, 12573-12582.	1.7	8
3459	Development of novel inorganic yellowish-tacao color pigments, RbBi _{1-x} Ce _x (MoO ₄) ₂ (0 ≤ x ≤ 0.30): revealing its crystal structure and color properties. New Journal of Chemistry, 0, , .	1.4	0
3460	Electrical and magneto-transport in the 2D semiconducting MXene Ti ₂ CO ₂ . Journal of Materials Chemistry C, 2022, 10, 9062-9072.	2.7	5
3461	Two-Dimensional Cds/Sii ² Heterostructure with Low Carrier Recombination as a Promising Photocatalyst for Water Splitting. SSRN Electronic Journal, 0, , .	0.4	0
3462	Electronic Properties and Magnetostriction in Fe-Ga Alloy of D0 ₃ Structure. SSRN Electronic Journal, 0, , .	0.4	0
3463	Functional Partition of Fe and Ti Co-Doped G-C ₃ N ₄ for Photo-Fenton Degradation of OTC: Performance, Mechanism, and Dft Study. SSRN Electronic Journal, 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
3482	3d ^d transition metal doped two-dimensional SnTe: Modulation of thermoelectric properties. <i>Materials Today Communications</i> , 2022, 31, 103656.	0.9	2
3483	Melamine Self-assembly and Dehydrogenation on Ag(111) Studied by Tip-enhanced Raman Spectroscopy. <i>Journal of Chemical Physics</i> , 0, , .	1.2	1
3484	Strain Engineering of 2D-C ₃ N ₅ Monolayer and Its Application in Overall Water-Splitting: a Hybrid Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8436-8449.	1.5	5
3485	Effects of Conjugated Structure on Electronic and Transport Properties in Organic-inorganic Hybrid Superlattices Cd ₂ Se ₂ (C ₂ H ₄ N ₂) _{1/2} . <i>Journal of Physics Condensed Matter</i> , 2022, 34, .	0.7	2
3486	Bandgap Engineering in Novel Fluorite-type Rare Earth High-Entropy Oxides (RE ₄ HEOs) with Computational and Experimental Validation for Photocatalytic Water Splitting Applications. <i>Advanced Sustainable Systems</i> , 2022, 6, .	2.7	22
3487	Band Gap Engineering of Newly Discovered ZnO/ZnS Polytropic Nanomaterials. <i>Nanomaterials</i> , 2022, 12, 1595.	1.9	9
3488	Ferroelectric Transition of a Chiral Molecular Crystal BINOL TM 2DMSO. <i>Journal of the Physical Society of Japan</i> , 2022, 91, .	0.7	2
3489	Investigation of electronic and optical properties of Pb _x Sn _{1-x} O ₂ for optoelectronic applications: A TB-mBJ DFT approach. <i>Computational Condensed Matter</i> , 2022, 31, e00691.	0.9	0
3490	Atomistic explanation of failure mechanisms of thermoelectric type-VIII clathrate Ba ₈ Ga ₁₆ Sn ₃₀ . <i>Materials Today Communications</i> , 2022, 31, 103605.	0.9	0
3491	DFT calculation of intrinsic properties of magnetically hard phase Li ₂ FePt. <i>Journal of Magnetism and Magnetic Materials</i> , 2022, 556, 169347.	1.0	4
3492	Spin polarized study of alkaline earth-cubic lead perovskites (PbXO ₃ , X = Mg, Ca & Sr) for emerging spintronic technology. <i>Journal of Crystal Growth</i> , 2022, 590, 126699.	0.7	13
3493	Supercapacitance in graphene oxide materials modified with tetrapyrrole dyes: a mechanistic study. <i>Nanoscale</i> , 2022, 14, 8534-8547.	2.8	1
3494	Revealing superstructure ordering in Heusler alloys and its effect on structural, magnetic, and electronic properties. <i>Physical Review B</i> , 2022, 105, .	1.1	2
3495	Thermal Transport and Mechanical Properties of Layered Oxychalcogenides LaCuOX (X = S, Se, and Te). <i>ACS Applied Energy Materials</i> , 2022, 5, 6943-6951.	2.5	5
3496	Ab initio molecular dynamics simulations on the adsorption of 1-hydroxyethane-1,1-diphosphonic acid on the iron (100) surface. <i>New Journal of Chemistry</i> , 2022, 46, 11797-11803.	1.4	1
3497	Exploring the electronic properties of N-doped graphene on graphitic and pyridinic models and its interaction with K ⁺ ions using the DFTB method. <i>Australian Journal of Chemistry</i> , 2022, , .	0.5	0
3498	Kinetic square scheme in oxygen-redox battery electrodes. <i>Energy and Environmental Science</i> , 2022, 15, 2591-2600.	15.6	21
3499	Atomistic simulation of martensite decay. <i>Modelling and Simulation in Materials Science and Engineering</i> , 0, , .	0.8	0

#	ARTICLE	IF	CITATIONS
3500	High-pressure behavior of tetragonal barium carbodiimide, BaNCN. Journal of Alloys and Compounds, 2022, 918, 165632.	2.8	3
3501	Solid and Liquid Oxygen under Ultrahigh Magnetic Fields. Oxygen, 2022, 2, 152-163.	1.6	2
3502	Structural and magnetic properties of churchite-type REPO ₄ ·2H ₂ O materials. Journal of Solid State Chemistry, 2022, 312, 123261.	1.4	2
3503	Discovery of Peculiar Electronic Structures of Decavacancy $<i>V</i>₁₀$ in Silicon Crystal. Journal of the Physical Society of Japan, 2022, 91, .	0.7	1
3504	CdS/Si ₁₂ : A promising two-dimensional materials for photocatalytic water splitting. Results in Physics, 2022, 38, 105636.	2.0	3
3505	Selective and sensitive toxic gas-sensing mechanism in a 2D Janus MoSSe monolayer. Physical Chemistry Chemical Physics, 2022, 24, 15292-15304.	1.3	13
3506	Two-dimensional heterotriangulene-based manganese organic frameworks: bipolar magnetic and half semiconductors with perpendicular magnetocrystalline anisotropy. Nanoscale, 2022, 14, 8865-8874.	2.8	4
3507	Copper Oxide Modified Activated Carbon for Enhanced Adsorption Performance of Siloxane: An Experimental and Dft Study. SSRN Electronic Journal, 0, , .	0.4	0
3508	Benchmarking various types of partial atomic charges for classical all-atom simulations of metal-organic frameworks. Nanoscale, 2022, 14, 9466-9473.	2.8	5
3509	Functional Partition of Fe and Ti Co-Doped G-C ₃ N ₄ for Photo-Fenton Degradation of OTC: Performance, Mechanism, and Dft Study. SSRN Electronic Journal, 0, , .	0.4	0
3510	Upconversion Luminescence Thermal Enhancement and Emission Color Modulation of Liygeo:Er ³⁺ /Yb ³⁺ +Phosphors. SSRN Electronic Journal, 0, , .	0.4	0
3511	Disordered Rock-Salt Type Li ₂ TiS ₃ as Novel Cathode for LIBs: A Computational Point of View. Nanomaterials, 2022, 12, 1832.	1.9	5
3512	High-Pressure and High-Temperature Syntheses of Aluminum-Transition Metal Alloy Hydrides with the Aid of <i>in situ</i> Synchrotron Radiation X-ray Diffraction Technique. Nihon Kessho Gakkaishi, 2022, 64, 165-169.	0.0	0
3513	X-ray Diffraction Study of the Structure of Gamma-Irradiated Low-Density Polyethylene. High Energy Chemistry, 2022, 56, 175-179.	0.2	3
3514	Synthesis of Nickel-Zinc Ferrite Nanoparticles by the Sol-Gel Auto-Combustion Method: Study of Crystal Structural, Cation Distribution, and Magnetic Properties. Advances in Condensed Matter Physics, 2022, 2022, 1-14.	0.4	12
3515	PdAg/Ag(111) Surface Alloys: A Highly Efficient Catalyst of Oxygen Reduction Reaction. Nanomaterials, 2022, 12, 1802.	1.9	3
3516	Structural evolution of single-crystal RECrO ₃ (RE = Y, Eu-Lu) orthochromates. Journal of Solid State Chemistry, 2022, 313, 123298.	1.4	3
3517	Mixed Anion Semiconductor In ₈ S _{2.82} Te _{6.18} (Te ₂) ₃ . Inorganic Chemistry, 2022, 61, 9040-9046.	1.9	1

#	ARTICLE	IF	CITATIONS
3518	Half-Metals and Weyl Nodal Line Semimetals in Two-Dimensional Phthalocyanine-Based Metal Organic Frameworks with Ni ²⁺ –Fe Dual Metals. <i>Journal of Physical Chemistry C</i> , 0, , .	1.5	2
3519	NaV(SO ₄) ₂ /C, Na ₃ V(SO ₄) ₃ /C, and K ₂ VO(SO ₄) ₂ /C: three Li-free vanadium sulfate cathode materials for lithium-ion batteries. <i>Journal of Solid State Electrochemistry</i> , 2022, 26, 1627-1636.	1.2	1
3520	High-throughput first-principles study of physical properties of L12-Al ₃ M particles. <i>Materials Today Communications</i> , 2022, , 103748.	0.9	0
3521	2D lead free Ruddlesden-Popper phase perovskites as efficient photovoltaic materials: A first-principles investigation. <i>Computational Materials Science</i> , 2022, 211, 111545.	1.4	6
3522	Layered iron dichalcogenides with high ion mobility and capacity as promising anode materials for alkali metal-ion batteries: A first-principles study. <i>Computational Materials Science</i> , 2022, 211, 111523.	1.4	0
3523	Computational understanding role of vacancies and distortions in wurtzite ferroelectric memory materials: implications for device miniaturization. <i>Materials Advances</i> , 2022, 3, 5532-5539.	2.6	2
3524	Atomic step formation on porous ZnO nanobelts: remarkable promotion of acetone gas detection up to the parts per trillion level. <i>Journal of Materials Chemistry A</i> , 2022, 10, 13839-13847.	5.2	19
3525	Comparison Among Various Physical Properties of Perovskite Oxides Bamo ₃ (M = Ru, Os) for Predicting Potential Applications. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3526	<i>Ab initio</i> investigation of electronic structure and optical properties of IrSn ₄ . <i>RSC Advances</i> , 2022, 12, 17882-17888.	1.7	0
3527	Pressure and temperature stability boundaries of cubic SiC polymorphs: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16228-16236.	1.3	3
3528	Energy landscapes of pure and doped ZnO: from bulk crystals to nanostructures. <i>Frontiers of Nanoscience</i> , 2022, , 151-193.	0.3	6
3529	<i>Theoretical prediction of mechanics, transport, and thermoelectric properties of full Heusler compounds</i> < mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" > < mml:mrow > < mml:msub > < mml:mi > Na < /mml:mi > < mml:mn > 2 < /mml:mn > < /mml:mrow > and < mml:math		

#	ARTICLE	IF	CITATIONS
3536	Magnetic behavior of ordered DO3-type Fe ₃ Al Heusler alloy. <i>Materials Today: Proceedings</i> , 2022, 65, 157-162.	0.9	3
3537	HP "A code for the calculation of Hubbard parameters using density-functional perturbation theory. <i>Computer Physics Communications</i> , 2022, 279, 108455.	3.0	35
3538	Topological descriptor of thermal conductivity in amorphous Si. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	8
3539	Prominent Electrode Material for Na-, K-, and Mg-ion Batteries: 2D \hat{I}^2 -Sb Monolayer. <i>Energy & Fuels</i> , 2022, 36, 7087-7095.	2.5	16
3540	Room-Temperature Electrochemical Fluoride (De)insertion into CsMnFeF ₆ . <i>ACS Energy Letters</i> , 2022, 7, 2340-2348.	8.8	3
3541	Ni- and Co-Struvites: Revealing Crystallization Mechanisms and Crystal Engineering toward Applicational Use of Transition Metal Phosphates. <i>Crystal Growth and Design</i> , 2022, 22, 4305-4315.	1.4	10
3542	Centimeter-scale perovskite SrTaO ₂ N single crystals with enhanced photoelectrochemical performance. <i>Science Bulletin</i> , 2022, 67, 1458-1466.	4.3	6
3543	Cobalt Anti-MXenes as Promising Anode Materials for Sodium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 10298-10308.	1.5	8
3544	Assessing (Mo _{2/3} Sc _{1/3}) ₂ C and (Mo _{2/3} Sc _{1/3}) ₂ CT ₂ (T = $\hat{\nu}$ O, $\hat{\nu}$ OH, and $\hat{\nu}$ F) i-MXenes as High-Performance Electrode Materials for Lithium and Non-Lithium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 10273-10286.	1.5	5
3545	The Local Structure and Metal-Insulator Transition in a Ba ₃ Nb ₅ $\hat{\nu}$ xTi _x O ₁₅ System. <i>Materials</i> , 2022, 15, 4402.	1.3	4
3546	The Structural, Mechanical, Lattice Dynamical, and Thermal Properties of 3D Dirac Semimetals BaXBi (X=Cu, Ag, Au) from First-Principles Calculations. <i>Physica Status Solidi (B): Basic Research</i> , 0, , 2200132.	0.7	1
3547	Structural and Electrical Properties of Annealed Ge ₂ Sb ₂ Te ₅ Films Grown on Flexible Polyimide. <i>Nanomaterials</i> , 2022, 12, 2001.	1.9	4
3548	Machine learning molecular dynamics simulations toward exploration of high-temperature properties of nuclear fuel materials: case study of thorium dioxide. <i>Scientific Reports</i> , 2022, 12, .	1.6	10
3549	Lattice Anharmonicity in BiS ₂ -Based Layered Superconductor RE(O,F)BiS ₂ (RE =) Tj ETQq _{1,1} 0.784 ₂ 14 rgBT (C	0.7	2
3550	Structural diversity and unusual valence states in compressed Na-Hg system. <i>Computational Materials Science</i> , 2022, 211, 111561.	1.4	0
3551	High-pressure synthesis and superconductivity of the novel laves phase BaIr ₂ . <i>Intermetallics</i> , 2022, 148, 107643.	1.8	5
3552	First principles modeling of CO ₂ adsorption on (100), (010), and (001) surfaces of wollastonite for applications in enhanced rock weathering. <i>Surface Science</i> , 2022, 724, 122143.	0.8	2
3553	Machine learning potentials of kaolinite based on the potential energy surfaces of CGA and meta-CGA density functional theory. <i>Applied Clay Science</i> , 2022, 228, 106596.	2.6	6

#	ARTICLE	IF	CITATIONS
3554	Nanoemulsification synthesis route for obtaining highly efficient Ag ₃ PO ₄ photocatalytic nanomaterial. Journal of the Serbian Chemical Society, 2022, 87, 1285-1296.	0.4	0
3555	Electronic structure and interface contact of two-dimensional van der Waals boron phosphide/Ga ₂ SSe heterostructures. RSC Advances, 2022, 12, 19115-19121.	1.7	4
3556	Luminescence study of alkaline earth aluminate-based nanophosphors. , 2022, , 327-355.		0
3557	A First-Principles Study: Three Novel N-Rich Barium~Nitrogen Compounds at High Pressures. SSRN Electronic Journal, 0, , .	0.4	0
3558	An All-Heusler Alloy Magnetic Tunneling Junction with Low Resistance Area Product and High Magnetocrystalline Anisotropy: A Dft Study. SSRN Electronic Journal, 0, , .	0.4	0
3559	Towards a relationship between photoluminescence emissions and photocatalytic activity of Ag ₂ SeO ₄ : combining experimental data and theoretical insights. Dalton Transactions, 2022, 51, 11346-11362.	1.6	5
3560	A First-Principles Study: Three Novel N-Rich Barium~Nitrogen Compounds at High Pressures. SSRN Electronic Journal, 0, , .	0.4	0
3561	Understanding the Role of Charge Storage Mechanisms in the Electrochromic Switching Kinetics of Metal Oxide Nanocrystals. Chemistry of Materials, 2022, 34, 5621-5633.	3.2	13
3562	First-Principles Core Spectroscopy of LiCoO ₂ and CoO ₂ . Journal of Physical Chemistry C, 2022, 126, 10949-10956.	1.5	1
3563	Li-Rich Mn-Mg Layered Oxide as a Novel Ni-Co-Free Cathode. Advanced Functional Materials, 2022, 32, .	7.8	13
3564	Large and Uniform Single Crystals of MoS ₂ Monolayers for ppb-Level NO ₂ Sensing. ACS Applied Nano Materials, 2022, 5, 9415-9426.	2.4	44
3565	First-Principles Investigation of the Structural, Elastic and Thermodynamic Properties of CaRu ₂ X ₂ (X=P, As) under Pressure. Journal of Superconductivity and Novel Magnetism, 0, , .	0.8	0
3566	Electronic and Magnetic Properties of 2D/3D MnB: An Ab-initio & Monte Carlo Study. Hittite Journal of Science & Engineering, 2022, 9, 103-110.	0.2	0
3567	On the structures and luminescent properties of Eu ³⁺ doped Li ₂ CaGeO ₄ , Ca ₂ GeO ₄ and Ca ₅ Ge ₃ O ₁₁ compounds. Luminescence, 0, , .	1.5	1
3568	Influence of ion irradiation-induced defects on phase formation and thermal stability of Ti _{0.27} Al _{0.21} N _{0.52} coatings. Acta Materialia, 2022, 237, 118160.	3.8	7
3569	Large-Area Uniaxial-Oriented Growth of Free-Standing Thin Films at the Liquid~Air Interface with Millimeter-Sized Grains. ACS Nano, 2022, 16, 11802-11814.	7.3	1
3570	An experimental analysis of the correlation between electronic structure and room temperature magnetism in Cu-doped CoFe ₂ O ₄ spinel ferrite. Applied Physics A: Materials Science and Processing, 2022, 128, .	1.1	4
3571	Studies on the variation of structural and thermodynamic properties of charge coupled substituted Na _x Eu _{1-x} Ca _{10-2x} (PO ₄) ₆ F ₂ solid solutions (x=0.5 to2.0). Journal of Alloys and Compounds, 2022, , 166331.	2.8	1

#	ARTICLE	IF	CITATIONS
3572	Copper oxide modified activated carbon for enhanced adsorption performance of siloxane: An experimental and DFT study. <i>Applied Surface Science</i> , 2022, 601, 154200.	3.1	5
3573	Halide perovskites as disposable epitaxial templates for the phase-selective synthesis of lead sulfochloride nanocrystals. <i>Nature Communications</i> , 2022, 13, .	5.8	16
3574	First principle study of the electronic and structural properties of NaFeAs superconductor. <i>Materials Today: Proceedings</i> , 2022, 66, 3349-3354.	0.9	0
3575	Study of high-temperature electrical conductivity and thermoelectric performance in $Mg_{2-x}Si_{0.35-x}Sn_{0.65}Ge_x$ ($x=0.04$ and $x=0, 0.05$) intermetallic alloys. <i>Journal of Materials Science: Materials in Electronics</i> , 2022, 33, 17842-17854.		
3576	Absence of topological $\hat{\Gamma}_2$ -antimonene and growth of $\hat{\Gamma}_\pm$ -antimonene on noble metal Ag(111) and Cu(111) surfaces. <i>Physical Review Materials</i> , 2022, 6, .	0.9	4
3577	Structural and elastic behaviour of aragonite at high-pressure: A contribution from first-principle simulations. <i>Computational Materials Science</i> , 2022, 212, 111600.	1.4	3
3578	Phase transitions and ferroelectricity of perovskite layered Sr ₂ Nb ₂ O ₇ ceramics. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 169, 110888.	1.9	4
3579	Thermal transport properties of anisotropic materials RbCaX (X = As, Sb) with strong anharmonicity. <i>Computational Materials Science</i> , 2022, 213, 111618.	1.4	8
3580	Structural transformation and magnetic properties of (Fe _{0.7} Co _{0.3}) ₂ B alloys doped with 5d elements: A combined first-principles and experimental study. <i>Journal of Alloys and Compounds</i> , 2022, 921, 166047.	2.8	1
3581	Tuning of carrier concentration and superconductivity in high-entropy-alloy-type metal telluride (Ag _{1-x} Sn _x PbBi)(1-)/4In Te. <i>Journal of Alloys and Compounds</i> , 2022, 920, 166013.	2.8	4
3582	Mechanochemistry-driven engineering of OD/3D heterostructure for designing highly luminescent CsPbBr ₃ perovskites. <i>Nature Communications</i> , 2022, 13, .	5.8	21
3583	Study on Stability and Elastic Properties of $\hat{\Gamma}_2$ -TiX (X=Nb, Ta) Alloys From First-Principles Calculations. <i>Frontiers in Materials</i> , 0, 9, .	1.2	0
3584	Strain-tunable pure \hat{H} conduction in one-atom-thick hexagonal boron nitride for high-energy-density fuel cells. <i>Chemical Engineering Journal</i> , 2022, 450, 138223.	6.6	3
3585	Layered potassium calcium phosphate with multiple exchangeable cations for Sr(II) and Co(II) removal from water. <i>Separation and Purification Technology</i> , 2022, 299, 121789.	3.9	6
3586	Towards targeted electronic properties of two-dimensional BaTiO ₃ films by tailoring surface structures: A first-principles study. <i>Applied Surface Science</i> , 2022, 602, 154377.	3.1	2
3587	Topochemical Synthesis of LiCoF ₃ with a High-Temperature LiNbO ₃ -Type Structure. <i>Inorganic Chemistry</i> , 2022, 61, 11746-11756.	1.9	0
3588	Calculated Elasticity of Al-Bearing Phase D. <i>Minerals (Basel, Switzerland)</i> , 2022, 12, 922.	0.8	2
3589	Optoelectronic properties of bilayer van der Waals WSe ₂ /MoSi ₂ N ₄ heterostructure: A first-principles study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 144, 115429.	1.3	5

#	ARTICLE	IF	CITATIONS
3590	Hidden Structural and Superconducting Phase Induced in Antiperovskite Arsenide SrPd ₃ As. <i>Inorganic Chemistry</i> , 2022, 61, 12149-12154.	1.9	1
3591	First-Principles Exploration of the Interface Characteristic between Cnt and Inorganic Lead-Free Perovskites Cs _n X ₃ (X = Cl, Br, I). <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
3592	Thermal enhancing effect of upconversion luminescence in Er ³⁺ /Yb ³⁺ co-doped Cs ₃ BiSr(P ₂ O ₇) ₂ phosphors. <i>Dalton Transactions</i> , 2022, 51, 12352-12361.	1.6	5
3593	Emission Enhancement and Energy Transfers in YV _{0.5} P _{0.5} O ₄ Nanoparticles Codoped with Eu ³⁺ and Bi ³⁺ Ions. <i>Inorganic Chemistry</i> , 2022, 61, 12237-12248.	1.9	3
3594	Upconversion thermal enhancement of ² H _{11/2} $\hat{\nu}^1$ ⁴ I _{15/2} of Er ³⁺ and blue emission of impurity Tm ³⁺ in Sr ₃ (PO ₄) ₂ :Er ³⁺ /Yb ³⁺ . <i>International Journal of Applied Ceramic Technology</i> , 0, , .	1.1	2
3595	Importance of Sugar-Phosphate Backbone and Counterions to First-Principles Modeling of Nucleobases. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5744-5751.	1.2	2
3596	High-pressure behavior and phase transition of jadarite, a promising B and Li mineral commodity. <i>Journal of the American Ceramic Society</i> , 2022, 105, 7011-7021.	1.9	3
3597	Ge-Containing Oxide-Ion Conductors with CaEu ₂ Ge ₃ O ₁₀ -Type Structure Discovered by the Bond-Valence Method and Experiments. <i>Inorganic Chemistry</i> , 2022, 61, 12327-12336.	1.9	0
3598	Two-dimensional B ₂ C as a potential anode material for Mg-ion batteries with extremely high theoretical capacity. <i>Scientific Reports</i> , 2022, 12, .	1.6	5
3599	Functionalization of Two-Dimensional Coordination Polymer in Small Organic Matter Removal from Organic Wastewater. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2022, 32, 3488-3495.	1.9	0
3600	Structure and electronic properties of amorphous strontium titanate. <i>Physical Review Materials</i> , 2022, 6, .	0.9	2
3601	Na ₃ H(ZnH ₄) Antiperovskite: A Large Octahedral Distortion with an Off-Centering Hydride Anion Coupled to Molecular Hydride. <i>Chemistry of Materials</i> , 2022, 34, 6815-6823.	3.2	8
3602	Regulating Electronic Conductivity at Cathode Interface for Low-Temperature Halide-Based All-Solid-State Batteries. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	9
3603	Effects of Ga Substitution on the Local Structure of Na ₂ Zn ₂ TeO ₆ . <i>Inorganic Chemistry</i> , 2022, 61, 13067-13076.	1.9	3
3604	Enhanced Stability of the Multiferroic Phase in Cr-Doped γ -Type Hexaferrite Single Crystals. <i>Physical Review Applied</i> , 2022, 18, .	1.5	2
3605	Enhanced Stability of the Multiferroic Phase in Cr-Doped γ -Type Hexaferrite Single Crystals. <i>Physical Review Applied</i> , 2022, 18, .	1.5	2
3605	Indication of a Systematic Charge Distribution Change in Bi _{0.5} Pb _{0.5} MO ₃ (M: 3d Transition Metal). <i>Inorganic Chemistry</i> , 2022, 61, 12822-12827.	1.9	0
3606	First-principles calculations to investigate switching from semiconducting to metallic with enhanced mechanical and optoelectronic properties of CsPbCl ₃ under pressure. <i>International Journal of Materials Research</i> , 2022, 113, 833-846.	0.1	2
3607	Ultrafast modification of the electronic structure of a correlated insulator. <i>Physical Review Research</i> , 2022, 4, .	1.3	8

#	ARTICLE	IF	CITATIONS
3608	Development of Copper Nanoparticle Conjugated Chitosan Microparticle as a stable source of 2nm copper nanoparticle effective against Methicillin-resistant Staphylococcus aureus. Pharmaceutical Nanotechnology, 2022, 10, .	0.6	0
3609	Facile synthesis of zinc hydroxyfluoride nanobelt and effect of hexamethylenetetramine for growth direction. Journal of Asian Ceramic Societies, 2022, 10, 697-702.	1.0	3
3610	Dehydrochlorination of PCDDs on SWCN-Supported Ni10 and Ni13 Clusters, a DFT Study. Molecules, 2022, 27, 5074.	1.7	1
3612	Lattice instability, anharmonicity and Raman spectra of BaO under high pressure: A first principles study. Journal of Physics and Chemistry of Solids, 2022, 170, 110967.	1.9	2
3613	Novel boronâ€rich aluminum nitride advanced ceramic materials. International Journal of Applied Ceramic Technology, 2023, 20, 174-189.	1.1	4
3614	High temperature stability and transport characteristics of hydrogen in alumina via multiscale computation. International Journal of Hydrogen Energy, 2022, , .	3.8	1
3615	LED-pumped intense red luminescence based on Ba2LaTaO6: Mn4+ double perovskite phosphor. Ceramics International, 2022, 48, 36140-36148.	2.3	12
3616	Vibrational and structural properties of the $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{R} \langle \text{mml:mi} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Fe} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$		

#	ARTICLE	IF	CITATIONS
3628	On the assignment of quartz-like LiAlSi ₂ O ₆ - SiO ₂ solid solutions in dental lithium silicate glass-ceramics: Virgilite, high quartz, low quartz or stuffed quartz derivatives?. <i>Dental Materials</i> , 2022, 38, 1558-1563.	1.6	6
3629	Direct decomposition of NO over 8MR in high silica Cu-LTA zeolite: A DFT study on reaction mechanisms, thermodynamics and kinetics. <i>Molecular Catalysis</i> , 2022, 530, 112602.	1.0	0
3630	Mapping of the degradation processes at bifunctional O ₂ gas diffusion electrode for aqueous alkaline metal-air batteries. <i>Journal of Power Sources</i> , 2022, 546, 231879.	4.0	3
3631	Charge conduction mechanism and non-debye type relaxation in LaCrO ₃ perovskite orthochromite. <i>Materials Chemistry and Physics</i> , 2022, 290, 126522.	2.0	8
3632	A single-phase white emitting nanophosphor with refined crystal structure and extremely luminescent characteristics for WLEDs and latent fingerprint detection. <i>Materials Chemistry and Physics</i> , 2022, 290, 126619.	2.0	8
3633	Pressure-induced lattice dynamical stability and superconductivity of ternary pentahydride $\langle \text{MgNiH}_5 \rangle$. <i>International Journal of Energy Research</i> , 2022, 46, 24064-24073.	2.2	2
3634	First-principles exploration of the interface characteristic between CNT and inorganic lead-free perovskites CsSnX ₃ (X=Cl, Br, I). <i>Materials Today Communications</i> , 2022, 33, 104524.	0.9	1
3635	Fast proton and water transport in ceramic membrane-based magic-angle graphene. <i>Water Research</i> , 2022, 225, 119076.	5.3	1
3636	Equilibrium fractionation of S, Fe, and Ni isotopes in Fe-Ni sulfides: A first-principles investigation. <i>Chemical Geology</i> , 2022, 610, 121100.	1.4	0
3637	First-principles calculations to investigate structural, elastic, electronic, thermodynamic, and thermoelectric properties of CaPd ₃ B ₄ O ₁₂ (B=Ti, V) perovskites. <i>Results in Physics</i> , 2022, 42, 105977.	2.0	54
3638	Strategy to weaken the oxygen adsorption on single-atom catalysts towards oxygen-involved reactions. <i>Materials Today Advances</i> , 2022, 16, 100280.	2.5	3
3639	First-principles investigation on electronic structures and energetic characteristics of $\hat{1}^3/\hat{1}^3$ tilt grain boundaries in $\hat{1}^3$ -TiAl intermetallic. <i>Intermetallics</i> , 2022, 151, 107723.	1.8	5
3640	Site-dependent mechanical properties of 3d transition metal-doped MnV intrinsic ductile intermetallic: First-principles and data mining study. <i>Computational Materials Science</i> , 2022, 215, 111801.	1.4	1
3641	Enhanced chemical durability of polymer electrolyte membrane fuel cells by crown ether grafted carbon nanotube. <i>Journal of Alloys and Compounds</i> , 2022, 928, 167227.	2.8	4
3642	Trapping mechanism of metastable $\hat{1}^2$ -Ga disclosed by its lattice stability optimization and nucleation behavior exploration. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022, 79, 102475.	0.7	1
3643	Effects of short-range order on phase equilibria and opto-electronic properties of ternary alloy Zn _x Cd _{1-x} Te. <i>Solar Energy Materials and Solar Cells</i> , 2022, 248, 111971.	3.0	1
3644	de Haas-van Alphen effect and the first-principles study of the possible topological stannide Cu ₃ Sn. <i>Journal of Alloys and Compounds</i> , 2022, 928, 167017.	2.8	0
3645	First-principles calculation on effects of oxygen vacancy on $\hat{1}^\pm$ -MnO ₂ and $\hat{1}^2$ -MnO ₂ during oxygen reduction reaction for rechargeable metal-air batteries. <i>Journal of Alloys and Compounds</i> , 2022, 926, 166929.	2.8	9

#	ARTICLE	IF	CITATIONS
3664	Unveiling the HER and ORR activity origin of isolated Co sites supported on N-doped carbon. MATEC Web of Conferences, 2022, 363, 01001.	0.1	0
3665	First-principles study of two-dimensional C-silicyne nanosheet as a promising anode material for rechargeable Li-ion batteries. Physical Chemistry Chemical Physics, 2022, 24, 20274-20281.	1.3	4
3666	Introduction to Molecular Dynamics Simulations. Lecture Notes in Applied and Computational Mechanics, 2022, , 1-19.	2.0	16
3667	Applying the HSAB design principle to the 3.5 V-class all-solid-state Li-ion batteries with a chloride electrolyte. Journal of Materials Chemistry A, 2022, 10, 20756-20760.	5.2	3
3668	Theoretical Consideration of Side Reactions between the VS₄; Electrode and Carbonate Solvents in Lithium-metal Polysulfide Batteries. Electrochemistry, 2022, 90, 107002-107002.	0.6	2
3669	Band alignment at Pt/PtFE interface: XPS experiment and first-principles calculation. , 2022, , .		1
3670	Prediction of Stable Silver Fluorides. Journal of Physical Chemistry C, 2022, 126, 15057-15063.	1.5	1
3671	High-efficiency photocatalyst based on a MoSiGeN ₄ /SiC heterojunction. Journal of Materials Science, 2022, 57, 16404-16417.	1.7	7
3672	Double-Bilayer polar nanoregions and Mn antisites in (Ca, Sr) ₃ Mn ₂ O ₇ . Nature Communications, 2022, 13, .	5.8	3
3673	Effect of radiation and substitution of Ce ⁴⁺ at Zr site in Y ₄ Zr ₃ O ₁₂ using collision cascades: a molecular dynamics simulation study. Journal of Nuclear Science and Technology, 2023, 60, 415-424.	0.7	1
3674	Urea Production on Metal-free Dual Silicon Doped C ₉ N ₄ Nanosheet Under Ambient Conditions by Electrocatalysis: A First Principles Study. ChemPhysChem, 0, , .	1.0	3
3675	Synergetic storage of ammonia over Al quantum dots embedded graphene sheets: A first principles perspective. International Journal of Hydrogen Energy, 2022, 47, 36873-36885.	3.8	1
3676	Hybrid improper ferroelectricity in A-cation ordered perovskite BaSrBi ₂ O ₆ . Journal of the Korean Physical Society, 0, , .	0.3	1
3677	Strong Dzyaloshinskii-Moriya interaction in monolayer $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{CrI} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle$ on metal substrates. Physical Review B, 2022, 106, .		
3678	Single- and Multilayers of Alkali Metal Atoms inside Graphene/MoS ₂ Heterostructures: A Systematic First-Principles Study. Journal of Physical Chemistry C, 2022, 126, 15558-15564.	1.5	4
3679	Synthesis, structural and physical properties of new ternary metal-rich phosphides M ₃ Ge ₂ P (M = Mo) Tj ETQq1 1 0.784314 rgBT /Overlo	1.4	4
3680	BaCO ₃ Nanoparticles-Modified Composite Cathode with Improved Electrochemical Oxygen Reduction Kinetics for High-Performing Ceramic Fuel Cells. Catalysts, 2022, 12, 1046.	1.6	4
3681	Magnetic properties and evolution of magnetoresistance effect in Pr _{0.75} Na _{0.05} K _{0.20} Mn _{1-x} FexO ₃ with \$0le xle\$ 0.04. Applied Physics A: Materials Science and Processing, 2022, 128, .	1.1	1

#	ARTICLE	IF	CITATIONS
3682	Uniaxial strain induced anisotropic bandgap engineering in freestanding BiFeO ₃ films. <i>APL Materials</i> , 2022, 10, .	2.2	2
3683	Role of orientational disorder in ZSM-22 in the adsorption of SO ₂ . <i>Molecular Physics</i> , 2022, 120, .	0.8	1
3684	Structural investigation and sonophotocatalytic properties of the solid solutions Sr(Mo _{1-x} W _x)O ₄ crystals synthesized by the sonochemical method. <i>Journal of Materials Science: Materials in Electronics</i> , 2022, 33, 22127-22152.	1.1	1
3685	Cu ⁺ Au nanoparticles produced by the aggregation of gas-phase metal atoms for CO oxidation. <i>Aggregate</i> , 2022, 3, .	5.2	9
3686	Superstructure Variation and Improved Cycling of Anion Redox Active Sodium Manganese Oxides Due to Doping by Iron. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	13
3687	Color coordination of emerald on CIE color space based on first-principles calculations. <i>Optical Materials: X</i> , 2022, 16, 100184.	0.3	1
3688	Structural and Electronic Properties of Cu ₃ InSe ₄ . <i>Crystals</i> , 2022, 12, 1310.	1.0	0
3689	Development of a dielectrically consistent reference interaction site model combined with the density functional theory for electrochemical interface simulations. <i>Physical Review Materials</i> , 2022, 6, .	0.9	4
3690	Structure-Property Relations of Nickel and Cobalt Substituted Yttrium Aluminum Garnets as Catalyst Materials for Dry Reforming of Methane. <i>Chemie-Ingenieur-Technik</i> , 0, , .	0.4	1
3691	Chemically exfoliated nanosheets of Bi ₂ O ₃ . <i>JPhys Materials</i> , 2022, 5, 044004.	1.8	1
3692	Structural characterization, phase analysis and electrochemical hydrogen storage studies on new pyrochlore SmRETi ₂ O ₇ (RE = Dy, Ho, and Yb) microstructures. <i>Ceramics International</i> , 2023, 49, 253-263.	2.3	55
3693	Crystal Structure of Bi ₃ Ca ₂ P ₂ O ₇ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 0, , .	0.6	2
3694	Influence of Inorganic Layer Thickness on Methylammonium Dynamics in Hybrid Perovskite Derivatives. <i>Chemistry of Materials</i> , 2022, 34, 8316-8323.	3.2	4
3695	Rietveld refinement, luminescence and catalytic study of as-synthesized and Dy ³⁺ -doped cubic Y ₂ O ₃ nanopowder prepared by citrate mediated sol-gel technique. <i>Journal of Nanoparticle Research</i> , 2022, 24, .	0.8	1
3696	Microstructure control and its observation of rapid solidification Cu-La alloy for the development of fluoride-ion batteries. <i>Journal of Alloys and Compounds</i> , 2022, , 167447.	2.8	1
3698	Magnetic Properties of Layered Hybrid Organic-Inorganic Metal-Halide Perovskites: Transition Metal, Organic Cation and Perovskite Phase Effects. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	11
3699	Computational studies on defect chemistry and Li-ion conductivity of spinel-type LiAl ₅ O ₈ as coating material for Li-metal electrode. <i>Scientific Reports</i> , 2022, 12, .	1.6	3
3700	A First-principles Study: Three Novel N-Rich Barium Nitrogen Compounds at High Pressures. <i>Results in Physics</i> , 2022, 42, 106030.	2.0	4

#	ARTICLE	IF	CITATIONS
3701	Features of Ni/Co Ordering in the $\text{LiNi}_{1-x}\text{Co}_x\text{PO}_4$ ($x = 0.3, 0.5, 0.7$) Crystal Structure. <i>Journal of Surface Investigation</i> , 2022, 16, 847-853.	0.1	0
3702	Anti-biofilm efficacy of green-synthesized ZnO nanoparticles on oral biofilm: In vitro and in silico study. <i>Frontiers in Microbiology</i> , 0, 13, .	1.5	9
3703	Tensile deformation and failure of tungsten single crystals. <i>International Journal of Refractory Metals and Hard Materials</i> , 2022, , 106013.	1.7	0
3704	The d-d transitions and ligand field parameters for $\text{Cr}^{3+}/\text{Co}^{2+}$ doped (Mg, Zn) Al_2O_4 : Multi-reference Ab initio investigations. <i>Optical Materials: X</i> , 2022, 16, 100188.	0.3	0
3705	Determination of exchange integrals and effect of cationic site occupancy (8b/24d) on the structural and magnetic properties of nanocrystalline Mn-doped Gd_2O_3 . <i>Journal of Alloys and Compounds</i> , 2022, , 167475.	2.8	0
3706	Influence of misfit strain on the physical properties of Fe thin films. <i>Thin Solid Films</i> , 2022, 761, 139494.	0.8	1
3707	Intrinsic ultra-low lattice thermal conductivity in orthorhombic BiSi: An excellent thermoelectric material. <i>Journal of Alloys and Compounds</i> , 2022, 929, 167347.	2.8	5
3708	Effects of Bi substitution on electroresistance behaviours in $\text{La}_{0.8}\text{Bi}_{0.2}\text{MnO}_3$ manganites. <i>Materials Chemistry and Physics</i> , 2022, 292, 126790.	2.0	6
3709	Enhanced polymerization interface of Ni_2P nanowires toward high-rate and durable cathode for alkaline Ni-Zn batteries. <i>Journal of Power Sources</i> , 2022, 550, 232170.	4.0	11
3710	Inducing magnetism in thermoelectric half-Heusler alloy NbCoSb through doping of Co/Mn metal for spin-caloritronics applications. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 171, 111025.	1.9	4
3711	STUDI TEORITIS SIFAT STRUKTUR DAN ELEKTRONIK MATERIAL TITANIUM DIOKSIDA DENGAN KALKULASI TEORI FUNGSIONAL KERAPATAN. , 2021, 2, 46-51.		0
3712	Effects of iron substitution and anti-site disorder on crystal structures, vibrational, optical and magnetic properties of double perovskites $\text{Sr}_{2-x}\text{Fe}_x\text{Ni}_x\text{TeO}_6$. <i>Dalton Transactions</i> , 0, .	1.6	1
3713	Two-Dimensional Nanomaterials Based Biosensors. <i>Topics in Applied Physics</i> , 2022, , 767-778.	0.4	1
3714	Bayesian optimisation with transfer learning for NASICON-type solid electrolytes for all-solid-state Li-metal batteries. <i>RSC Advances</i> , 2022, 12, 30696-30703.	1.7	4
3716	Atomic structure for AlN grown on different plane orientation of sapphire via numerical study. <i>Microelectronics International</i> , 2023, 40, 46-52.	0.4	0
3717	Electronic Properties and Chemical Bonding in V_2FeSi and Fe_2VSi Heusler Alloys. <i>Crystals</i> , 2022, 12, 1546.	1.0	3
3718	Theoretical Study of Oxygen Reduction Reaction Mechanism in Metal-Free Carbon Materials: Defects, Structural Flexibility, and Chemical Reaction. <i>ACS Nano</i> , 2022, 16, 16394-16401.	7.3	13
3719	Simultaneous influence of Mg^{2+} and Sc^{3+} co-doping on upconversion luminescence and optical thermometry in $\text{F}^{2-}\text{NaYF}_4: \text{Yb}^{3+}/\text{Ho}^{3+}$ microphosphor. <i>Journal of Alloys and Compounds</i> , 2023, 934, 167732.	2.8	9

#	ARTICLE	IF	CITATIONS
3720	Structural and Elastic Behaviour of Sodalite Na ₈ (Al ₆ Si ₆ O ₂₄)Cl ₂ at High-Pressure by First-Principle Simulations. Minerals (Basel, Switzerland), 2022, 12, 1323.	0.8	2
3721	Study on Spectral Characteristics and Color Origin of Scheelite from Xuebaoding, Pingwu County, Sichuan Province, P.R. China. Minerals (Basel, Switzerland), 2022, 12, 1344.	0.8	1
3722	Griffiths-like phase, large magnetocaloric effect, and unconventional critical behavior in the NdSrCoFeO ₆ disordered double perovskite. Physical Review B, 2022, 106, .		5
3723	The Effects of Mo Partial Substitution at the Mn Site on Electroresistance Behaviour in La _{0.7} Ba _{0.3} Mn _{1-x} MoxO ₃ (x = 0, 0.01, 0.02, 0.03, 0.04) Manganites. Journal of Electronic Materials, 2023, 52, 237-250.		3
3724	Optical-Acoustic Phonon Hybridization Enhanced Thermoelectric Performance in a 1Tâ€² Phase OsTe ₂ Monolayer. ACS Applied Energy Materials, 2022, 5, 14513-14521.	2.5	6
3725	Quantum spin Hall effect from multiscale band inversion in twisted bilayer Bi ₂ Se ₃ . Physical Review Research, 2022, 4, .		
3726	Synthesis of rare-earth metal compounds through enhanced reactivity of alkali halides at high pressures. Communications Chemistry, 2022, 5, .	2.0	3
3727	Optimization of Biocatalytic Steps via Response Surface Methodology to Produce Immobilized Peroxidase on Chitosan-Decorated AZT Composites for Enhanced Reusability and Storage Stability. Catalysis Letters, 2023, 153, 2543-2557.	1.4	2
3728	Correlation between thermopower and carrier mobility in the thermoelectric semimetal Ta ₂ PdSe ₆ . Applied Physics Letters, 2022, 121, .	1.5	1
3729	Prediction of structural, electronic, and lattice dynamical properties of ABO ₃ [A = K, Rb, Cs; B = Sn, Sb] perovskite compounds. Physica B: Condensed Matter, 2023, 649, 414355.	1.3	9
3730	Computational Prediction and Experimental Realization of Earth-Abundant Transparent Conducting Oxide Ga-Doped ZnSb ₂ O ₆ . ACS Energy Letters, 2022, 7, 3807-3816.	8.8	5
3731	Electric field control of phonon angular momentum in perovskite BaTiO ₃ . Physical Review Materials, 2022, 6, .		
3732	Detailed Structural and Electrochemical Comparison between High Potential Layered P ₂ -NaMnNi and Doped P ₂ -NaMnNiMg Oxides. ACS Applied Energy Materials, 2022, 5, 13735-13750.	2.5	5
3733	Deposition of Horizontally Stacked Zn Crystals on Single Layer 1Tâ€²VSe ₂ for Dendrite-Free Zn Metal Anodes. Advanced Energy Materials, 2022, 12, .	10.2	11
3734	Ultraviolet and visible upconversion in Yb/Er-CaSiO ₃ Î²-wollastonite phosphors. Ceramics International, 2023, 49, 7489-7499.	2.3	3
3735	Accurate Electronic Properties and Intercalation Voltages of Olivine-Type Li-Ion Cathode Materials from Extended Hubbard Functionals. , 2022, 1, .		10
3736	Electronic topological transitions and mechanical properties of hafnium dioxide allotrope at high pressure: Evolutionary first-principles techniques. Physica B: Condensed Matter, 2022, , 414456.	1.3	0
3737	First-principles study of two-dimensional half-metallic ferromagnetism in NiXCl (X = S and Se) monolayer. AIP Advances, 2022, 12, 115105.	0.6	1

#	ARTICLE	IF	CITATIONS
3738	The negative thermal expansion behavior in Prussian blue analogue Zn ₃ [Fe(CN) ₆] ₂ : A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022, 453, 128493.	0.9	1
3739	Antimicrobial and Ion-exchange Properties of Layered KHSi ₂ O ₅ Compounds Prepared Using Amorphous Silicon Dioxide (a-SiO ₂) Blocks. <i>Journal of Ion Exchange</i> , 2022, 33, 112-117.	0.1	2
3740	Atomistic simulation of shear deformation at bcc-Fe grain boundary and precipitation strengthening by Cr ₂₃ C ₆ . <i>Materials Today Communications</i> , 2022, 33, 104711.	0.9	0
3741	Encapsulate lithium sulfide cathodes with carbon-doped MoS ₂ for fast kinetics in lithium-sulfur batteries, a theoretical study. <i>Acta Materialia</i> , 2023, 242, 118441.	3.8	7
3742	Enhanced photocatalytic toluene oxidation performance induced by two types of cooperative fluorine doping in polymeric carbon nitride with the first-principles calculations. <i>Journal of Colloid and Interface Science</i> , 2023, 630, 452-459.	5.0	4
3743	Electronic and transport properties of Heusler alloy based magnetic tunneling junctions: A first principles study. <i>Computational Materials Science</i> , 2023, 216, 111852.	1.4	3
3744	Combination of peroxymonosulfate and Fe(II) for enhanced degradation of sulfamethoxazole: The overlooked roles of high-valent iron species. <i>Chemical Engineering Journal</i> , 2023, 453, 139742.	6.6	22
3745	A DFT study on the stability and optoelectronic properties of Pb/Sn/Ge-based MA ₂ B(SCN) ₂ I ₂ perovskites. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
3746	Investigation of the effect of point defects on the Li-ion conductivity of Li ₃ InCl ₆ . <i>Dalton Transactions</i> , 0, , .	1.6	1
3747	Disordering in Fe ₃ Ga alloy of D0 ₃ structure: Effect on stability and magnetostriction. <i>Computational Materials Science</i> , 2023, 216, 111878.	1.4	0
3748	Functional partition of Fe and Ti co-doped g-C ₃ N ₄ for photo-Fenton degradation of oxytetracycline: Performance, mechanism, and DFT study. <i>Separation and Purification Technology</i> , 2023, 306, 122546.	3.9	32
3749	DFT crystal and electronic structure of the direct bandgap Cu _(1-x) NaxPF ₆ : (x = 0.125n, n = 1-7). <i>Journal of Physics and Chemistry of Solids</i> , 2023, 173, 111116.	1.9	0
3750	Effects of alloying elements (Cr, Fe and Mo) on the interfacial properties of ³ Ni(110)/TiC(110) in TiC-particles reinforced NMCs: First-principles study. <i>Optics and Laser Technology</i> , 2023, 158, 108870.	2.2	0
3751	Novel far-red emitting phosphor Mn ⁴⁺ -activated BaLaLiWO ₆ with excellent performance for indoor plant cultivation of light-emitting diodes. <i>Journal of Alloys and Compounds</i> , 2023, 934, 167927.	2.8	8
3752	Crystal and electronic structures of BiS ₂ -based compounds		

#	ARTICLE	IF	CITATIONS
3756	Libra: A modular software library for quantum nonadiabatic dynamics. <i>Software Impacts</i> , 2022, 14, 100445.	0.8	6
3757	Effects of Fluorinated Aromatic Spacer in Ag ⁺ Bi Double Perovskite for X-ray Detector. <i>Journal of Physical Chemistry C</i> , 2022, 126, 19417-19423.	1.5	6
3758	A thermo-kinetic investigation on the thermal degradation of polyvinyl chloride in the presence of magnetite and hematite. <i>Thermochimica Acta</i> , 2022, 718, 179390.	1.2	4
3759	Polarons in Rock-Forming Minerals: Physical Implications. <i>Condensed Matter</i> , 2022, 7, 68.	0.8	3
3760	Pressure-induced phase transition and band-gap decrease in semiconducting Na ₃ Bi(IO ₃) ₆ . <i>Results in Physics</i> , 2023, 44, 106156.	2.0	4
3761	Unraveling the low-temperature activity of Rh ⁺ CeO ₂ catalysts in CO oxidation: probing the local structure and Red-Ox transformation of Rh ³⁺ species. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2862-2874.	1.3	2
3762	Intense blue-emitting Yb/Tm-CaSiO ₃ wollastonite upconversion phosphors. <i>Optical Materials</i> , 2023, 135, 113326.	1.7	1
3763	Estimation of Gr ^{1/4} neisen Parameter of Layered Superconductor La _{0.5} F _{0.5} BiS ₂ Se _x ((x =) Tj ETQ ₁ 1 0.784314 rgBT	1.0	1
3764	Transport properties of As-F-based molecular magnetic tunnel junctions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2023, 457, 128570.	0.9	1
3765	Disordered spin gapless semiconducting CoFeCrGa Heusler alloy thin films on Si (100): experiment and theory. <i>Nanoscale</i> , 2022, 15, 337-349.	2.8	6
3766	Interstitial diffusion of hydrogen in M ₃ C (M=Cr, Mn, Fe). <i>Computational Materials Science</i> , 2023, 218, 111952.	1.4	1
3767	Effect of transition metals on the crystal field in CeCo _{0.4} Fe _{0.6} Ge ₃ . <i>Intermetallics</i> , 2023, 153, 107776.	1.8	1
3768	First-principles DFT study of structural, electronic and optical properties of Cu-doped TiO ₂ (112) surface for enhanced visible-light photocatalysis. <i>Computational Materials Science</i> , 2023, 218, 111952.	1.4	5
3769	Crystal structure, microstructure, and ultra-high energy storage properties of lead-free		

#	ARTICLE	IF	CITATIONS
3774	Optical and thermoelectric properties of square lattice phases of alkali halide compounds. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 174, 111142.	1.9	1
3775	First-principles study on CVD growth mechanism of 2D NbC on Cu(1 1 1) surface. <i>Applied Surface Science</i> , 2023, 613, 156086.	3.1	0
3776	Effect of Ho ³⁺ on structural and magnetic properties of the Sm _{3-x} HoxFe ₅ O ₁₂ ceramic system. <i>Materials Research Bulletin</i> , 2023, 160, 112127.	2.7	1
3777	Transport and thermoelectric properties of strongly anharmonic Full-Heusler compounds CsK ₂ M (M=As, Bi). <i>Materials Today Communications</i> , 2023, 34, 105134.	0.9	1
3778	Predicting the adsorption and reduction of NO ₂ on Sr-doped CeO ₂ (1 1 1) using first-principles calculations. <i>Applied Surface Science</i> , 2023, 612, 155896.	3.1	0
3779	Se-doped Li ₆ PS ₅ Cl and Li _{5.5} PS _{4.5} Cl _{1.5} with improved ionic conductivity and interfacial compatibility: a high-throughput DFT study. <i>Journal of Materials Chemistry C</i> , 2022, 10, 18294-18302.	2.7	2
3780	First-principles study on photoelectric properties of all-inorganic two-dimensional double perovskite Cs ₃ AgBiBr ₇ . <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3175-3181.	1.3	6
3781	A mechanism for aragonite to post-aragonite transition in MCO ₃ (M = Ca, Sr and Ba) carbonates: evidence of a hidden metastable polymorph. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 29205-29213.	1.3	2
3782	<i>Ab initio</i> methods for the computation of physical properties and performance parameters of electrochemical energy storage devices. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1476-1503.	1.3	3
3783	Conversion of Nastrophites to Fibrous Strontium Apatites and Their Crystallographic Characterization. <i>Crystals</i> , 2022, 12, 1705.	1.0	0
3784	A structural optimization algorithm with stochastic forces and stresses. <i>Nature Computational Science</i> , 2022, 2, 736-744.	3.8	4
3785	New $\hat{1}$ -NaFeO ₂ synthesis route for green sodium-ion batteries. <i>Green Materials</i> , 2023, 11, 115-124.	1.1	2
3786	Origin of enhanced dielectric and multiferroic properties in Pb-doped BaTiO ₃ ceramics. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, .	1.1	6
3787	Oxidation processes and thermal stability of actinolite. <i>Physics and Chemistry of Minerals</i> , 2022, 49, .	0.3	3
3788	Experimental and Theoretical Correlation of Modulated Architectures of $\hat{1}$ -Ag ₂ MoO ₄ Microcrystals: Effect of Different Synthesis Routes on the Morphology, Optical, Colorimetric, and Photocatalytic Properties. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2023, 33, 424-450.	1.9	9
3789	The First-Principles Study On The Investigation of Magnetic and Electronic Properties of Ga ₄ X ₃ Mn (X =) Tj ETQq1 1,0,784314,rgBT /Ove	0,1	0
3790	Ground-State Surface of All-Inorganic Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2022, 126, 21155-21161.	1.5	4
3791	Real-space obstruction in quantum spin Hall insulators. <i>Physical Review B</i> , 2022, 106, .	1.1	4

#	ARTICLE	IF	CITATIONS
3792	Crystallographic and Physicochemical Analysis of Bovine and Human Teeth Using X-ray Diffraction and Solid-State Nuclear Magnetic Resonance. <i>Journal of Functional Biomaterials</i> , 2022, 13, 254.	1.8	2
3793	Halogen's effect on the photoelectric properties of two-dimensional organic-inorganic hybrid perovskite (MTEA) ₂ MAPb ₂ X ₇ (X = Cl, Br, I) with a Ruddlesden-Popper structure. <i>Applied Physics Letters</i> , 2022, 121, .	1.5	5
3794	Non-destructive determination of the biotite crystal chemistry using Raman spectroscopy: how far we can go?. <i>European Journal of Mineralogy</i> , 2022, 34, 573-590.	0.4	4
3795	Surface Interactions and Nanoconfinement of Methane and Methane plus CO ₂ Revealed by High-Pressure Magic Angle Spinning NMR Spectroscopy and Molecular Dynamics. <i>Membranes</i> , 2022, 12, 1273.	1.4	4
3796	Creating superconductivity in WB ₂ through pressure-induced metastable planar defects. <i>Nature Communications</i> , 2022, 13, .	5.8	13
3797	On-Surface Synthesis of Chiral Graphene Nanoribbon Segments via the Quarter-Anthryl on Au(111) Surface. <i>Advanced Materials Interfaces</i> , 2023, 10, .	1.9	4
3798	The Local Coordination Effects on the Reactivity and Speciation of Active Sites in Graphene-Embedded Single-Atom Catalysts over Wide pH and Potential Range. <i>Nanomaterials</i> , 2022, 12, 4309.	1.9	3
3799	Anion-Dependent Polarization and Piezoelectric Power Generation in Hybrid Halide MAPbX ₃ (X = I, Br, and Cl) Thin Films with Out-of-Plane Structural Adjustments. <i>Advanced Science</i> , 2023, 10, .	5.6	4
3800	Nuclear and magnetic spin structure of the antiferromagnetic triangular lattice compound LiCrTe ₂ investigated by μ^+ SR, neutron and X-ray diffraction. <i>Scientific Reports</i> , 2022, 12, .	1.6	3
3801	Analyzing the physical properties of perovskite oxides BaMO ₃ (M = Ru, Os) for predicting potential applications. <i>Computational Condensed Matter</i> , 2023, 34, e00782.	0.9	5
3802	Remarkable thermoelectric performance of carbon-based schwarzites. <i>Advanced Composites and Hybrid Materials</i> , 2023, 6, .	9.9	16
3803	Cerium(III) Niobate Layered Perovskites: Abnormal Optical Absorption Modulations by Tuning of B-Site Composition and Perovskite Layer Charge Control. <i>Inorganic Chemistry</i> , 2022, 61, 20636-20646.	1.9	1
3804	Cu(I)/Cu(II) Creutz-Taube Mixed-Valence 2D Coordination Polymers. <i>Small Methods</i> , 0, , 2201166.	4.6	1
3805	High-Pressure Synthesis and Magnetic and Electrical Properties of Fe-Doped Bi ₃ Re ₃ O ₁₁ and Bi ₃ Os ₃ O ₁₁ . <i>Inorganic Chemistry</i> , 2022, 61, 21148-21156.	1.9	4
3806	Perovskite grain wrapping by converting interfaces and grain boundaries into robust and water-insoluble low-dimensional perovskites. <i>Science Advances</i> , 2022, 8, .	4.7	20
3807	Electrocatalytic Biomass Upgrading of Furfural using Transition-Metal Borides via Density Functional Theory Investigation. <i>Small</i> , 2023, 19, .	5.2	8
3808	Metal Single-Site Molecular Complex-MXene Heteroelectrocatalysts Interspersed Graphene Nanonetwork for Efficient Dual-Task of Water Splitting and Metal-Air Batteries. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	16
3809	Fast Ion Transport in Li-Rich Alloy Anode for High-Energy-Density All Solid-State Lithium Metal Batteries. <i>Advanced Functional Materials</i> , 0, , 2209715.	7.8	7

#	ARTICLE	IF	CITATIONS
3810	Computational study of adsorption of magnesium polysulfides on VS ₄ magnesium sulfur batteries. <i>Materials Today: Proceedings</i> , 2023, 76, 352-358.	0.9	1
3811	Prediction of bipolar VSi_2 and VGe_2 monolayers with high Curie temperature and strong magnetocrystalline. <i>Physical Review B</i> , 2022, 106, .	1.1	4
3812	Understanding effect of distortions and vacancies in wurtzite AlScN ferroelectric memory materials: Vacancy-induced multiple defect state types and relaxation dependence in transition energy levels. <i>AIP Advances</i> , 2022, 12, .	0.6	2
3813	Revisiting the Nature of Chemical Bonding in Chalcogenides to Explain and Design their Properties. <i>Advanced Materials</i> , 2023, 35, .	11.1	32
3814	Toward Uniaxially Textured CsPbI ₂ Perovskite Thin Films with Twin Domains by Potassium Incorporation. <i>ACS Energy Letters</i> , 2023, 8, 699-706.	8.8	1
3815	Facile low-energy and open-air synthesis of mixed-cation perovskite quantum dots for high-performance solar cells. <i>Chemical Engineering Journal</i> , 2023, 457, 141107.	6.6	4
3816	Thermoelectric transport properties of orthorhombic RbBaX (X = Sb, Bi) with strong anharmonicity. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
3817	Model-based deconvolution for particle analysis applied to a through-focus series of HAADF-STEM images. <i>Microscopy (Oxford, England)</i> , 2023, 72, 368-380.	0.7	1
3818	Interstitial Electron-Induced Topological Molecular Crystals. , 2023, 2, .		1
3819	Investigation of Structure, Ionic Conductivity, and Electrochemical Stability of Halogen Substitution in Solid-State Ion Conductor Li ₃ YBr _x Cl _{6-x} . <i>Journal of Physical Chemistry C</i> , 2023, 127, 125-132.	1.5	7
3820	Structure and Luminescence Studies of a Ce ³⁺ -Activated Ba ₅ La ₃ MgAl ₃ O ₁₅ Green-Emitting Phosphor. <i>Inorganic Chemistry</i> , 2023, 62, 1250-1256.	1.9	14
3821	A plausible investigation of low dimensional magnetism in a 3D spin system PrVO ₄ . <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	2
3822	Giant caloric effects in charge spin lattice coupled transition-metal oxides. <i>Journal of Materials Chemistry A</i> , 2023, 11, 12695-12702.	5.2	3
3823	Structure and lithium insertion in oxides of molybdenum. <i>APL Materials</i> , 2023, 11, .	2.2	4
3824	Screening chloride Li-ion conductors using high-throughput force field molecular dynamics. <i>Journal of the American Ceramic Society</i> , 2023, 106, 3035-3044.	1.9	3
3825	Critical resolved shear stresses for slip and twinning in Mg-Y-Ca alloys and their effect on the ductility. <i>International Journal of Plasticity</i> , 2023, 162, 103525.	4.1	18
3826	Investigation of enhanced Am selectivity for Eu in solvent extraction using a BTPPhen ligand substituted with halogen. <i>RSC Advances</i> , 2023, 13, 2476-2482.	1.7	0
3827	Detection of H ₂ S, HF and H ₂ pollutant gases on the surface of penta-PdAs ₂ monolayer using DFT approach. <i>Scientific Reports</i> , 2023, 13, .	1.6	13

#	ARTICLE	IF	CITATIONS
3828	Origin of Vanadium Site Sequential Oxidation in $KxVPO_4F$. Chemistry of Materials, 2023, 35, 617-627.	3.2	2
3829	Spin-Lattice and Magnetoelectric Couplings Enhanced by Orbital Degrees of Freedom in Polar Multiferroic Semiconductors. Physical Review Letters, 2023, 130, .	2.9	5
3830	Weyl-Kondo semimetal behavior in the chiral structure phase of $Ce_{1-x}Mn_x$. Physical Review Materials, 2023, 7, .	0.3	1
3831	Microsupercapacitors with low particle thermal conductivity in natural superlattice materials.		

#	ARTICLE	IF	CITATIONS
3846	Mixed Sulfur/Selenium Anions Weaken Electron-Vibrational Interaction in $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ Photoabsorber. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 107-115.	2.1	1
3847	Double Paddle-Wheel Enhanced Sodium Ion Conduction in an Antiperovskite Solid Electrolyte. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	11
3848	Systematic Theoretical Study of CO Activation over Clean and Potassium-Modified Transition Metals. <i>Journal of Physical Chemistry C</i> , 2023, 127, 265-278.	1.5	1
3849	Crystal and Electronic Structures of New Two Dimensional 3-NH ₃ -PyPbX ₄ Haloplumbate Materials. <i>Materials</i> , 2023, 16, 353.	1.3	1
3850	Molecular adsorption on coinage metal subnanoclusters: A DFT + D ₃ investigation. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	1
3851	Sc_2X_3	0.9	3
3852	Re-investigating the structure-property relationship of the solid electrolytes $\text{Li}_3\text{In}_2\text{ZrCl}_6$ and the impact of In-Zr substitution. <i>Journal of Materials Chemistry A</i> , 0, , .	5.2	3
3853	Mo(V) system	1.1	2
3854	Crystallographic at non-ambient conditions and physical properties of the synthesized double-perovskites $\text{Sr}_2(\text{Co}_{1-x}\text{Fex})\text{TeO}_6$. <i>Dalton Transactions</i> , 0, , .	1.6	1
3855	Halide-based perovskites in photonics: From photocatalysts to highly efficient optoelectronic devices. , 2023, , 547-600.		1
3856	Ferro-piezoelectricity in emerging Janus monolayer BMX_2 (M = Ga, In and X = S, Se): <i>ab initio</i> investigations. <i>Nanoscale Advances</i> , 2023, 5, 1425-1432.	2.2	5
3857	Charge Manipulation in a Series of π -Stacked Pillared-Layer Frameworks by Tuning Electron Donation Ability of Building Blocks. <i>Crystal Growth and Design</i> , 2023, 23, 1238-1246.	1.4	0
3858	Non-centrosymmetric Weyl semimetal state and strain effect in the twisted-brick phase transition metal monochalcogenides. <i>Nanoscale</i> , 2023, 15, 2882-2890.	2.8	1
3859	Pyridinic Dominance N-Doped Graphene: A Potential Material for SO_2 Gas Detection. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1112-1123.	1.1	5
3860	Probing the molecular-level energy absorption mechanism and strategic sequencing of graphene/Al composite laminates under high-velocity ballistic impact of nano-projectiles. <i>Applied Surface Science</i> , 2023, 629, 156502.	3.1	5
3861	Strong anharmonicity and high thermoelectric performance of cubic thallium-based fluoride perovskites TlXF_3 (X = Hg, Sn, Pb). <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 5776-5784.	1.3	6
3862	Learning local equivariant representations for large-scale atomistic dynamics. <i>Nature Communications</i> , 2023, 14, .	5.8	86
3863	About the Impact of Defect Phases on the Thermoelectric Properties of $\text{Cr}_3\text{S}_4\text{Se}$.	1.6	2

#	ARTICLE	IF	CITATIONS
3864	Interstitial Zinc Boosted Light Tunability, Afterglow, and Ultrabright White Emission in Zinc Germanate (Zn_2GeO_4). ACS Applied Electronic Materials, 2023, 5, 1286-1294.	2.0	10
3865	Multicomponent solid solution with pyrochlore structure. Boletin De La Sociedad Espanola De Ceramica Y Vidrio, 2023, 62, 515-526.	0.9	1
3866	Synthesis of new non-covered and silica-covered $Y_{0.9}Tm_{0.1-x}Yb_xVO_4$ nanophosphors with emission in the visible and NIR ranges. Journal of Luminescence, 2023, 257, 119708.	1.5	0
3867	Role of defect engineering in revealing the electronic and sensing applications of Janus WSSe monolayer. Journal of Materials Chemistry C, 2023, 11, 4219-4234.	2.7	2
3868	Can magnetotransport properties provide insight into the functional groups in semiconducting MXenes?. Nanoscale, 2023, 15, 10254-10263.	2.8	1
3869	BN Diamane-like Quasicrystal Based on 30° Twisted H-BN Bilayers and Its Approximants: Features of the Atomic Structure and Electronic Properties. Crystals, 2023, 13, 421.	1.0	1
3870	Electronic Structure and Photocatalytic Water Splitting Application of a New Type II g-ZnO/Ga ₂ SSe van der waals Heterostructure. Catalysis Letters, 2024, 154, 601-609.	1.4	0
3871	Catalyst regeneration and multicycle growth of high purity and yield semiconducting single-walled carbon nanotubes. Chemical Engineering Journal, 2023, 462, 142272.	6.6	2
3872	Enhancement of the $Na_2FePO_4F@gC_3N_4$ electrochemical performance in view of its implementation in sodium-ion batteries. Solid State Ionics, 2023, 392, 116167.	1.3	3
3873	Investigation of the effect of F-doping on the solid-electrolyte property of Li_3InCl_6 . Journal of Power Sources, 2023, 567, 232962.	4.0	6
3874	Green synthesized ZnO/NiO heterostructures based quick responsive LPG sensor for the detection of below LEL with DFT calculations. Results in Surfaces and Interfaces, 2023, 11, 100103.	1.0	3
3875	Ion kinetic energy- and ion flux-dependent mechanical properties and thermal stability of (Ti,Al)N thin films. Acta Materialia, 2023, 250, 118864.	3.8	9
3876	Chemically modified graphene sheets as potential sensors for organophosphate compounds(pesticide): A DFT study. Applied Surface Science, 2023, 619, 156745.	3.1	4
3877	Design of a highly efficient Cu-based catalyst with two functional areas: The role of CuO and oxygen vacancies in Fenton-like system. Chemical Engineering Journal, 2023, 464, 142420.	6.6	9
3878	Enhancing quantum capacitance of iron sulfide supercapacitor through defect-engineering: A first-principles calculation. Electrochimica Acta, 2023, 449, 142235.	2.6	3
3879	On the enhanced performance of Pt-based high-entropy alloys catalyst during water-gas shift reaction: A density functional theory study. Applied Surface Science, 2023, 623, 157023.	3.1	3
3880	Structural and mechanical properties of Al/TiC interface with vacancies: First-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2023, 471, 128786.	0.9	1
3881	Discerning the crystal structure and engineering the optoelectronic properties through substitution of divalent cations (M= Zn, N = Ge) in $C_3H_3MNI_3$ for solar cell applications. Materials Science in Semiconductor Processing, 2023, 160, 107449.	1.9	3

#	ARTICLE	IF	CITATIONS
3882	Efficiently electrochemical CO ₂ reduction on molybdenum-nitrogen-carbon catalysts with optimized p-block axial ligands. <i>Chemical Engineering Science</i> , 2023, 273, 118638.	1.9	2
3883	Boosting thermoelectric performance of HfSe ₂ monolayer by selectivity chemical adsorption. <i>Journal of Colloid and Interface Science</i> , 2023, 639, 14-23.	5.0	0
3884	On ionic transport through pores in a borophene-graphene membrane. <i>Materials Today Chemistry</i> , 2023, 30, 101512.	1.7	2
3885	Electrocatalytic nitrogen reduction on defective graphene modulated from single atom catalyst to aluminium clusters. <i>Applied Surface Science</i> , 2023, 623, 157024.	3.1	3
3886	Electron density distribution and microstructural spherical harmonic calculation of BaTiO ₃ powders and ceramics. <i>Journal of Solid State Chemistry</i> , 2023, 322, 123988.	1.4	2
3887	Investigation on transport properties and anomalously heat-carrying optical phonons in KXY (X = Ca, Tl) ETQq1 1 0,784314 rgBT /Over	2.5	0
3889	Structures and electron states of (4,4)CNT-graphene hybrid system through DFTB investigation. <i>Materials Today Communications</i> , 2023, 35, 105576.	0.9	0
3890	Design, synthesis and investigating the interaction of novel s-triazine collector with pyrite surface: A DFT-D3+U and experimental studies. <i>Surfaces and Interfaces</i> , 2023, 38, 102820.	1.5	1
3891	Efficacy of pyrostitpnite (Ag ₃ SbS ₃) mineral as thermoelectric material: A first principles study. <i>Materials Science in Semiconductor Processing</i> , 2023, 162, 107513.	1.9	3
3892	Thermoelectric performance of Zintl compound KMgBi with layered structure. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 178, 111308.	1.9	3
3893	Dittmarite-type magnesium phosphates for highly efficient capture of Cs ⁺ . <i>Journal of Hazardous Materials</i> , 2023, 453, 131385.	6.5	2
3895	Strong anharmonic phonon scattering and superior thermoelectric properties of Li ₂ NaBi. <i>Materials Today Physics</i> , 2023, 31, 100990.	2.9	11
3896	Uniaxial Negative Thermal Expansion in an Orthorhombic Superconductor CoZr ₃ . <i>Journal of the Physical Society of Japan</i> , 2023, 92, .	0.7	2
3897	Dynamic structural and microstructural responses of a metal-organic framework type material to carbon dioxide under dual gas flow and supercritical conditions. <i>Journal of Applied Crystallography</i> , 2023, 56, 222-236.	1.9	2
3898	First principles study on structural, vibrational, electronic and elastic properties of 2D alkaline-earth carbides as a metallic material. <i>Synthetic Metals</i> , 2023, 293, 117281.	2.1	0
3899	Metal borohydrides as ambient-pressure high- T_c superconductors. <i>Physical Review B</i> , 2023, 107, .		
3900	Effect of sintering temperature on re-distribution of cations, electronic structure and tuning of optical band gap and ferromagnetism in Mn _{0.1} Co _{0.9} Fe ₂ O ₄ spinel ferrites. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2023, 78, 281-295.	0.7	0
3901	Band gap engineering of anatase TiO ₂ by ambipolar doping: A first principles study. <i>Materials Chemistry and Physics</i> , 2023, 299, 127467.	2.0	4

#	ARTICLE	IF	CITATIONS
3902	Strong quartic anharmonicity, ultralow thermal conductivity, high band degeneracy and good thermoelectric performance in Na ₂ TlSb. <i>Npj Computational Materials</i> , 2023, 9, .	3.5	18
3903	New High-Pressure Structures of Transition Metal Carbonates with O ₃ Câ€“CO ₃ Orthooxalate Groups. <i>Symmetry</i> , 2023, 15, 421.	1.1	2
3904	Evolution of Martensite Tetragonality in High-Carbon Steels Revealed by In Situ High-Energy X-Ray Diffraction. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2023, 54, 1083-1100.	1.1	3
3905	Spin-Gapless Semiconductors and Quantum Anomalous Hall Effects of Tetraazaphthalene-Based Two-Dimensional Transition-Metal Organic Frameworks on Spintronics and Electrocatalysts for CO ₂ Reduction. <i>ACS Applied Electronic Materials</i> , 2023, 5, 1243-1251.	2.0	4
3906	Effect of Hydrostatic Pressure on Lone Pair Activity and Phonon Transport in Bi ₂ O ₂ S. <i>ACS Applied Energy Materials</i> , 2023, 6, 2401-2411.	2.5	4
3908	$\frac{1}{2} \frac{V_{MoO_2}}{V_{MoO_3}}$	1.0	1
3909	Enhanced emission intensity in (Li ⁺ /Ca ²⁺ /Bi ³⁺) ions co-doped NaLa(MoO ₄) ₂ : Dy ³⁺ phosphors and their Judd-Ofelt analysis for WLEDs applications. <i>Methods and Applications in Fluorescence</i> , 2023, 11, 024001.	1.1	2
3910	Firstâ€“Principles Density Functional Theory and Machine Learning Technique for the Prediction of Water Adsorption Site on PtPdâ€“Based Highâ€“Entropyâ€“Alloy Catalysts. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	3
3911	Study on low hydrostatic pressure-dependent optoelectronic, mechanical, and anisotropic properties of heavy thallium perovskites TlPbX ₃ (X=â€“Cl, Br). <i>Journal of Materials Research</i> , 2023, 38, 2007-2017.	1.2	4
3912	Electrochemical Conversion of Cu Nanowire Arrays into Metal-Organic Frameworks HKUST-1. <i>Journal of the Electrochemical Society</i> , 2023, 170, 022506.	1.3	1
3913	Thermal and Electronic Properties of Ba ₂ MnSe ₃ . <i>Inorganic Chemistry</i> , 2023, 62, 3555-3561.	1.9	3
3914	Glassy atomic vibrations and blurry electronic structures created by local structural disorders in high-entropy metal telluride superconductors. <i>Materials Today Physics</i> , 2023, 32, 101019.	2.9	2
3916	Grain Boundary Phases in NbFeSb Halfâ€“Heusler Alloys: A New Avenue to Tune Transport Properties of Thermoelectric Materials. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	20
3917	Chiral and Catalytic Effects of Site-Specific Molecular Adsorption. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2072-2077.	2.1	1
3918	Linear and Nonlinear Optical Properties of Quadrupolar Bithiophenes and Cyclopentadithiophenes as Fluorescent Oxygen Photosensitizers. <i>Photochem</i> , 2023, 3, 127-154.	1.3	0
3919	Immunomodulatory natural polysaccharides: An overview of the mechanisms involved. <i>European Polymer Journal</i> , 2023, 188, 111935.	2.6	7
3920	Abnormal thermal expansion coefficients in (Nd _{1-x} Dy _x) ₂ Zr ₂ O ₇ pyrochlore: The effect of low-lying optical phonons. <i>Journal of Advanced Ceramics</i> , 2023, 12, 1001-1014.	8.9	2
3921	Unraveling the effects of inter-site Hubbard interactions in spinel Li-ion cathode materials. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9061-9072.	1.3	2

#	ARTICLE	IF	CITATIONS
3922	Origin of oxygen-redox and transition metals dissolution in Ni-rich $\text{Li}_x\text{Ni}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ cathode. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	3
3923	Geometric frustration of Jahn–Teller order in the infinite-layer lattice. <i>Nature</i> , 2023, 615, 237-243.	13.7	14
3924	Ferroelectric switching pathways and domain structure of SrBi_2O_9 from first principles. <i>Physical Review B</i> , 2023, 107, .	1.1	1
3925	Theoretical Study on the Role of Solvents in Lithium Polysulfide Anchoring on Vanadium Disulfide Facets for Lithium–Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4416-4424.	1.5	3
3926	Coupling between Charge Density Wave Ordering and Magnetism in $\text{Ho}_2\text{Ir}_3\text{Si}_5$. <i>Chemistry of Materials</i> , 2023, 35, 1980-1990.	3.2	6
3927	Theoretical analysis of electrochromism of Ni-deficient nickel oxide “ from bulk to surfaces. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7974-7985.	1.3	1
3928	Influence of Nitrogen Substitution on the Electronic Structure of Ti_2O_3 : Insights into the Doping-Induced Insulator–Metal Transition. <i>Physica Status Solidi (B): Basic Research</i> , 2023, 260, .	0.7	0
3929	Enhancing spin splitting by symmetry and molecular orbital hybridization in VO_2 . <i>Computational Materials Science</i> , 2023, 222, 112100.	1.4	2
3930	Ambipolar Electrochemistry of Pre-Intercalated $\text{Ti}_3\text{C}_2\text{T}_x$ MXene in Ionic Liquid Electrolyte. <i>Batteries and Supercaps</i> , 2023, 6, .	2.4	2
3931	Understanding the Role of Entropy in High Entropy Oxides. <i>Journal of the American Chemical Society</i> , 2023, 145, 5991-6006.	6.6	51
3932	Development of $\text{NaY}_9\text{Si}_6\text{O}_{26}:\text{Yb}^{3+}$ phosphors with high thermal stability for NIR anti-counterfeiting: study of its crystal structure and luminescent properties. <i>RSC Advances</i> , 2023, 13, 7597-7602.	1.7	0
3933	Magnetoelastic Coupling and Cryogenic Magnetocaloric Effect in Two-Site Disordered CdSrCoFeO_6 Double Perovskite. <i>Chemistry of Materials</i> , 2023, 35, 2439-2455.	3.2	7
3934	Charge Trapping and Emission Properties in CAAC-IGZO Transistor: A First-Principles Calculations. <i>Materials</i> , 2023, 16, 2282.	1.3	2
3935	Pressure-induced structural phase transitions in natural monazite. <i>Physical Review B</i> , 2023, 107, .	1.1	0
3936	Near ultraviolet excitable cyan-green phosphors of $\text{Ba}_6\text{La}_2\text{Al}_3\text{ScO}_{15}:\text{Ce}^{3+}$ and $\text{Ba}_6\text{La}_2\text{Al}_3\text{ScO}_{15}:\text{Ce}^{3+},\text{Tb}^{3+}$: investigations on the crystal structure, site assignment of Ce^{3+} and Tb^{3+} ions, and an energy transfer process from Ce^{3+} to Tb^{3+} . <i>Dalton Transactions</i> , 2023, 52, 5252-5264.	1.6	2
3937	Nd-doped NASICON-type nanophosphors for near-infrared excitation and emission. <i>Journal of Asian Ceramic Societies</i> , 2023, 11, 239-249.	1.0	0
3938	Investigations of Vacancy-Assisted Selective Detection of NO_2 Molecules in Vertically Aligned SnS_2 . <i>ACS Sensors</i> , 2023, 8, 1357-1367.	4.0	11
3939	Hot carrier relaxation dynamics in non-stoichiometric CdSe quantum dots: computational insights. <i>Journal of Materials Chemistry A</i> , 2023, 11, 8256-8264.	5.2	4

#	ARTICLE	IF	CITATIONS
3940	Facile Tailoring of Surface Terminations of MXenes by Doping Nb Element: Toward Extraordinary Pseudocapacitance Performance. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 15367-15376.	4.0	6
3941	Synthesis and Characterization of a Trigonal Layered Compound AgInS_2 . <i>ACS Omega</i> , 2023, 8, 11288-11292.	1.6	0
3942	A van der Waals Heterostructure with an Electronically Textured Moiré Pattern: $\text{PtSe}_2/\text{PtTe}_2$. <i>ACS Nano</i> , 2023, 17, 5913-5920.	7.3	1
3943	Impact of Erbium Doping in the Structural and Magnetic Properties of the Anisotropic and Frustrated SrYb_2O_4 Antiferromagnet. <i>Crystals</i> , 2023, 13, 529.	1.0	0
3944	Structural mapping and tuning of mixed halide ions in amorphous sulfides for fast Li-ion conduction and high deformability. <i>Journal of Materials Chemistry A</i> , 2023, 11, 7457-7467.	5.2	2
3945	Synthesis and Structure of RUB-58: An Almost Ordered, Highly Crystalline Member of the ZSM-48 Family of Zeolites. <i>Crystal Growth and Design</i> , 2023, 23, 2770-2781.	1.4	1
3946	SCIENTIA SINICA Terrae, 2023, 53, 714-722.	0.1	0
3947	Ab initio study on the electromechanical response of Janus transition metal dihalide nanotubes. <i>European Physical Journal B</i> , 2023, 96, .	0.6	2
3948	Local structural features of medium-entropy garnet with ultra-long cycle life. <i>Matter</i> , 2023, 6, 1530-1541.	5.0	8
3949	Effect of Oxygen Reduction Reaction on Pt/Pd ₃ Fe (111) Alloy Electrocatalyst: A DFT Study. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 3170-3178.	0.1	0
3950	New hydrous phases in the $\text{Al}_2\text{O}_3\text{-SiO}_2\text{-H}_2\text{O}$ system under the mantle transition zone conditions. <i>Science China Earth Sciences</i> , 2023, 66, 730-737.	2.3	0
3951	Upconversion luminescence thermal enhancement from visible to near infrared and improving temperature sensitivity under high temperature using a second-harmonic generation response. <i>Materials Today Chemistry</i> , 2023, 29, 101487.	1.7	1
3952	Factors controlling heteroepitaxial phase formation at intermetallic- Al_3Sc /liquid interfaces. <i>Journal of Applied Physics</i> , 2023, 133, 124902.	1.1	0
3953	Catalytic Activity Maps for Alloy Nanoparticles. <i>Journal of the American Chemical Society</i> , 2023, 145, 7352-7360.	6.6	10
3954	Exploring oxygen non-stoichiometry in presumably stoichiometric double perovskites: the case study for $\text{LaCu}_{0.5}\text{Mn}_{0.5}\text{O}_3$. <i>Acta Materialia</i> , 2023, 250, 118872.	3.8	1
3955	Silicate Dissolution Mechanism from Metakaolinite Using Density Functional Theory. <i>Nanomaterials</i> , 2023, 13, 1196.	1.9	8
3956	Luminescence-structure relationships in solids doped with Bi^{3+} . <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 11027-11054.	1.3	8
3957	Magnetic properties and muon localization in Cr_2S_3 . <i>Journal of Physics: Conference Series</i> , 2023, 2462, 012006.	0.3	0

#	ARTICLE	IF	CITATIONS
3958	Magnetic nature of wolframite MgReO_4 . Journal of Physics: Conference Series, 2023, 2462, 012037.	0.3	3
3959	Quasi-2D FCC lithium crystals inside defective bi-layer graphene: insights from first-principles calculations. Materials Today Energy, 2023, 34, 101293.	2.5	2
3960	Nanosized Ti-Based Perovskite Oxides as Acid-Base Bifunctional Catalysts for Cyanosilylation of Carbonyl Compounds. ACS Applied Materials & Interfaces, 2023, 15, 17957-17968.	4.0	4
3961	Crystal structure, magnetism, and thermoelectric properties of $\text{Nd}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$ (0.1 ≤ x ≤ 0.9). Japanese Journal of Applied Physics, 2023, 62, 080501.	0.8	0
3962	DFT+U functional derived to explicitly address the flat plane condition. Physical Review B, 2023, 107, 115401.	1.1	5
3963	Electronic and structural properties of $\text{Y}_6\text{Pt}_{13}\text{X}_4$, site occupancy variants of the $\text{Ba}_6\text{Na}_{16}\text{N}$ nitride (X = Al, Ga). Dalton Transactions, 2023, 0, 11500.	1.6	0
3964	Crystal structure and electronic properties of low-dimensional hexamethylenediaminium lead halide perovskites. Dalton Transactions, 2023, 0, 11500.	1.6	1
3965	Role of Non-covalent Interaction toward Conductivity in a One-Dimensional Tube-like Silver-Thiolate Structure. Crystal Growth and Design, 2023, 23, 3164-3170.	1.4	1
3966	Engineering d-p orbital hybridization through regulation of interband energy separation for durable aqueous Zn/VO ₂ (B) batteries. Chemical Engineering Journal, 2023, 464, 142711.	6.6	6
3967	Insights into the Electrochemical Production of Hydrogen Peroxide over Single-Atom Co-N-C Catalysts with the Introduction of Carbon Vacancy Defect near the Co-N ₄ Site. Journal of Physical Chemistry Letters, 2023, 14, 3658-3668.	2.1	4
3968	Hexagonal Tungsten Bronze $\text{H}_{0.25}\text{Cs}_{0.25}\text{Nb}_{2.5}\text{W}_{2.5}\text{O}_{14}$ as a Negative Electrode Material for Li-Ion Batteries. Chemistry of Materials, 2023, 0, 11500.	3.2	0
3969	Monitoring the melting behavior of boron nanoparticles using a neural network potential. Physical Chemistry Chemical Physics, 2023, 25, 12841-12853.	1.3	3
3970	Crystal structure, dielectric and magnetic properties of $(1-x)\text{BaTiO}_3-x\text{BaFe}_2\text{O}_9$ (x = 0.50, 0.60, 0.70) multiferroic composites. Applied Physics A: Materials Science and Processing, 2023, 129, 11000.	1.1	6
3971	Computational Design of Cation-Disordered $\text{Li}_3\text{Ta}_2\text{O}_5$ with Fast Ion Diffusion Dynamics and Rich Redox Chemistry for a High-Rate Li-Ion Battery Anode Material. Chemistry of Materials, 2023, 0, 11500.	3.2	0
3972	Cation disorder dominates the defect chemistry of high-voltage $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ (LMNO) spinel cathodes. Journal of Materials Chemistry A, 2023, 11, 13353-13370.	5.2	7
3973	Magnetic phase diagrams of the pyrochlore-based magnets: Landau theory. Journal of Magnetism and Magnetic Materials, 2023, 0, 11500.	1.0	0
3974	An atomistic modeling study of high-throughput RVO_3 (R=La, Nd) perovskites for efficient solar energy conversion materials. Physica B: Condensed Matter, 2023, 660, 414879.	1.3	4
3975	Prediction of wide-gap topological insulating phase in metastable BiTeI. Applied Physics Express, 2023, 0, 11500.	1.1	0

#	ARTICLE	IF	CITATIONS
3976	An outlook into the magnetic and magnetocaloric properties of Cr _{1.3} Fe _{0.7} O ₃ . Physica Status Solidi (B): Basic Research, 0, , .	0.7	0
3977	Mixed-valent Nb boosted the electrochemical performance of K ₃ Nb ₆ P ₄ O ₂₆ @C anode material for lithium-ion batteries. Journal of Alloys and Compounds, 2023, 953, 170160.	2.8	0
3978	Designing dithiolene and bis(iminothiolato)-based 1D metal-organic-frameworks for electrocatalytic hydrogen evolution reaction. Theoretical Chemistry Accounts, 2023, 142, .	0.5	2
3979	Reversible Electrochemical Lithium Cycling in a Vanadium(IV)- and Niobium(V)-Based Wadsleyâ€Roth Phase. Chemistry of Materials, 0, , .	3.2	0
3980	Evaluation of adsorption and mechanical strength of 13X zeolite mixtures with phyllosilicate binders using molecular dynamics simulation and positron annihilation spectroscopy. Chemical Engineering Science, 2023, 276, 118744.	1.9	1
3981	Effect of particle microstructure and the role of proton on the lithium insertion properties of HTiNbO ₅ electrode material. Electrochimica Acta, 2023, , 142432.	2.6	0
3982	Phonon-mediated strong coupling between a three-dimensional topological insulator and a two-dimensional antiferromagnetic material. Physical Review Materials, 2023, 7, .	0.9	3
3983	Co-doped hydroxyapatite as photothermal catalyst for selective CO ₂ hydrogenation. Applied Catalysis B: Environmental, 2023, 333, 122790.	10.8	4
3984	Density functional theory investigation on the structural, mechanical, lattice dynamical and thermal properties of nodal-line semimetals CaAgX (X: P, As). Bulletin of Materials Science, 2023, 46, .	0.8	0
3985	Mechanism of Stoichiometrically Governed Titanium Oxide Brownian Tree Formation on Stepped Au(111). Journal of Physical Chemistry C, 0, , .	1.5	1
3986	Boosting heterogeneous catalyst discovery by structurally constrained deep learning models. Materials Today Chemistry, 2023, 30, 101541.	1.7	0
3987	9,10-phenanthrenequinone anchored on nitrogen-doped carbon nanotubes for symmetrical supercapacitors with enhanced performance. Journal of Materials Science: Materials in Electronics, 2023, 34, .	1.1	1
3988	$\text{P} : \text{Isovalent tuning of Mn-sublattice magnetic order. Physical Review B, 2023, 107, .}$	1.1	1
3989	Janus PdSTe nanosheet as promising contender for detection of volatile organic compounds (VOCs) in human breath: A first principles investigation. Chemical Engineering Journal, 2023, 466, 143101.	6.6	2
3990	On the anomalous high-pressure phase transition of inderite, MgB ₃ O ₃ (OH)5 \cdot 5H ₂ O. Solid State Sciences, 2023, , 107187.	1.5	0
4021	Catalysts: Platinum-free. , 2023, , .		0
4054	Impact of Temperature on Dielectric Properties of BiFeO ₃ Nanoparticles for PV Applications. , 2023, , .		1
4068	Molecular-scale synchrotron X-ray investigations of solid-liquid interfaces in lithium-ion batteries. , 2023, , .		0

#	ARTICLE	IF	CITATIONS
4122	Effect of different dopants on the structural and physical properties of In ₂ S ₃ thin films: a review. Journal of Materials Science, 2023, 58, 12143-12157.	1.7	1
4278	Basic guidelines of first-principles calculations for suitable selection of electrochemical Li storage materials: a review. Journal of Materials Chemistry A, 2023, 11, 24482-24518.	5.2	4
4430	Unravelling abnormal in-plane stretchability of two-dimensional metal-organic frameworks by machine learning potential molecular dynamics. Nanoscale, 2024, 16, 3438-3447.	2.8	0
4439	Photoinduced Novel Lattice Instability in SnSe. Springer Theses, 2023, , 77-99.	0.0	0
4441	Compact Boundary Matrix from a Polytopal Complex for Computing Persistent Homology. , 2023, , .		0