Isao Tanaka

List of Publications by Year
in descending order

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354 papers	30,907 citations	10956 71 h-index	5101 166 g-index
364 all docs	364 docs citations	364 times ranked	23741 citing authors

#	Article	IF	Citations
1	First principles phonon calculations in materials science. Scripta Materialia, 2015, 108, 1-5.	2.6	7,324
2	First-principles calculations of the ferroelastic transition between rutile-type and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaCl</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu high pressures. Physical Review B, 2008, 78, .	1.1	4,498
3	Distributions of phonon lifetimes in Brillouin zones. Physical Review B, 2015, 91, .	1.1	963
4	High-Density Electron Anions in a Nanoporous Single Crystal: [Ca24Al28O64]4+(4e-). Science, 2003, 301, 626-629.	6.0	744
5	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655
6	Band structure diagram paths based on crystallography. Computational Materials Science, 2017, 128, 140-184.	1.4	457
7	First-principles phonon calculations of thermal expansion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub Physical Review B, 2010, 81, .	1.1	429
8	Phonon-phonon interactions in transition metals. Physical Review B, 2011, 84, .	1.1	363
9	Energetics of native defects in ZnO. Journal of Applied Physics, 2001, 90, 824-828.	1.1	360
10	Prediction of Low-Thermal-Conductivity Compounds with First-Principles Anharmonic Lattice-Dynamics Calculations and Bayesian Optimization. Physical Review Letters, 2015, 115, 205901.	2.9	343
11	Crystal and electronic structures of superstructural Li1â^'x[Co1/3Ni1/3Mn1/3]O2 (0â‰¤xâ‰¤1). Journal of Power Sources, 2003, 119-121, 644-648.	4.0	316
12	Point defects in ZnO: an approach from first principles. Science and Technology of Advanced Materials, 2011, 12, 034302.	2.8	279
13	Prediction model of band gap for inorganic compounds by combination of density functional theory calculations and machine learning techniques. Physical Review B, 2016, 93, .	1.1	252
14	Machine learning with systematic density-functional theory calculations: Application to melting temperatures of single- and binary-component solids. Physical Review B, 2014, 89, .	1.1	243
15	Representation of compounds for machine-learning prediction of physical properties. Physical Review B, 2017, 95, .	1.1	220
16	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. Physical Review B, 2006, 73, .	1.1	218
17	Lithium Iron Borates as Highâ€Capacity Battery Electrodes. Advanced Materials, 2010, 22, 3583-3587.	11.1	218
18	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212

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19	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. Physical Review B, 2008, 78, .	1.1	210
20	Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis. Nature Communications, 2016, 7, 11962.	5.8	208
21	Interesting Physical Properties of the New Spinel Phase ofSi3N4andC3N4. Physical Review Letters, 1999, 83, 5046-5049.	2.9	205
22	Hot Isostatic Press Sintering and Properties of Silicon Nitride without Additives. Journal of the American Ceramic Society, 1989, 72, 1656-1660.	1.9	188
23	Calcium Concentration Dependence of the Intergranular Film Thickness in Silicon Nitride. Journal of the American Ceramic Society, 1994, 77, 911-914.	1.9	179
24	Accelerated Materials Design of Lithium Superionic Conductors Based on Firstâ€Principles Calculations and Machine Learning Algorithms. Advanced Energy Materials, 2013, 3, 980-985.	10.2	178
25	First-principles calculations of ELNES and XANES of selected wide-gap materials: Dependence on crystal structure and orientation. Physical Review B, 2004, 70, .	1.1	162
26	First-principles study on lithium removal from Li2MnO3. Journal of Power Sources, 2009, 189, 798-801.	4.0	158
27	Design and synthesis of a magnesium alloy for room temperature hydrogen storage. Acta Materialia, 2018, 149, 88-96.	3.8	157
28	Relativistic cluster calculation of ligand-field multiplet effects on cationL2,3x-ray-absorption edges ofSrTiO3,NiO, andCaF2. Physical Review B, 2001, 64, .	1.1	155
29	Pure H ^{â€“} conduction in oxyhydrides. Science, 2016, 351, 1314-1317.	6.0	155
30	Solid-State Chemistry and Electrochemistry of LiCo[sub 1/3]Ni[sub 1/3]Mn[sub 1/3]O[sub 2] for Advanced Lithium-Ion Batteries. Journal of the Electrochemical Society, 2004, 151, A1545.	1.3	154
31	Anharmonicity in the High-Temperature<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:math>Phase of SnSe: Soft Modes and Three-Phonon Interactions. Physical Review Letters, 2016, 117, 075502.	8.6	147
32	Structure and Stability of a Homologous Series of Tin Oxides. Physical Review Letters, 2008, 100, 045702.	2.9	146
33	Defect Chemistry in Layered LiMO₂ (M = Co, Ni, Mn, and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 187 3886-3894.	3.2	128
34	Cluster expansion method for multicomponent systems based on optimal selection of structures for density-functional theory calculations. Physical Review B, 2009, 80, .	1.1	116
35	XANES and ELNES in Ceramic Science. Journal of the American Ceramic Society, 2005, 88, 2013-2029.	1.9	111
36	Multiplet calculations of L_{2,3}x-ray absorption near-edge structures for 3d transition-metal compounds. Journal of Physics Condensed Matter, 2009, 21, 104208.	0.7	110

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37	Ab initiolattice dynamics and phase transformations ofZrO2. Physical Review B, 2005, 71, .	1.1	109
38	Role of Ti Antisitelike Defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 103, 185502.	2.9	109
39	Effects of Off-Stoichiometry of LiC₆ on the Lithium Diffusion Mechanism and Diffusivity by First Principles Calculations. Journal of Physical Chemistry C, 2010, 114, 2375-2379.	1.5	109
40	Accelerated discovery of cathode materials with prolonged cycle life for lithium-ion battery. Nature Communications, 2014, 5, 4553.	5.8	108
41	Electronic Structure of Lithium Nickel Oxides by Electron Energy Loss Spectroscopy. Journal of Physical Chemistry B, 2005, 109, 10749-10755.	1.2	106
42	First-principles XANES simulations of spinel zinc ferrite with a disordered cation distribution. Physical Review B, 2007, 75, .	1.1	105
43	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. Computer Physics Communications, 2017, 221, 221-234.	3.0	105
44	Antiferromagnetic superexchange via<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>states of titanium in EuTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>as seen from hybrid Hartree-Fock density functional calculations. Physical Review B, 2011, 83, .	1.1	104
45	Theoretical Formation Energy of Oxygen-Vacancies in Oxides. Materials Transactions, 2002, 43, 1426-1429.	0.4	101
46	Systematic Research on Insertion Materials Based on Superlattice Models in a Phase Triangle of LiCoO[sub 2]-LiNiO[sub 2]-LiMnO[sub 2]. Journal of the Electrochemical Society, 2004, 151, A1499.	1.3	101
47	Core-hole effects on theoretical electron-energy-loss near-edge structure and near-edge x-ray absorption fine structure of MgO. Physical Review B, 2000, 61, 2180-2187.	1.1	98
48	Pressure-induced phase transition in ZnO andZnOâ^'MgOpseudobinary system: A first-principles lattice dynamics study. Physical Review B, 2005, 72, .	1.1	98
49	Decomposition reactions forNaAlH4,Na3AlH6, and NaH: First-principles study. Physical Review B, 2005, 71, .	1.1	97
50	Room temperature ferromagnetism in Mn-doped Î³-Ga2O3 with spinel structure. Applied Physics Letters, 2006, 89, 181903.	1.5	97
51	First-principles multielectron calculations of NiL2,3NEXAFS and ELNES forLiNiO2and related compounds. Physical Review B, 2005, 72, .	1.1	94
52	Ab initiocharge transfer multiplet calculations on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn> and ELNES of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition metal oxides. Physical Review B, 2011, 83, .	1.1	94
53	Antiâ€ferrodistortiveâ€Like Oxygenâ€Octahedron Rotation Induced by the Oxygen Vacancy in Cubic SrTiO₃. Advanced Materials, 2013, 25, 86-90.	11.1	94
54	Prediction of spinel structure and properties of single and double nitrides. Physical Review B, 2001, 63, .	1.1	92

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55	Prediction of ground-state structures and order-disorder phase transitions in II-III spinel oxides: A combined cluster-expansion method and first-principles study. Physical Review B, 2006, 73, .	1.1	91
56	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. Journal of the American Ceramic Society, 2002, 85, 75-80.	1.9	90
57	Mechanism of electrical conductivity of transparentInGaZnO4. Physical Review B, 2000, 61, 1811-1816.	1.1	88
58	Reduced SnO2 surfaces by first-principles calculations. Applied Physics Letters, 2004, 84, 909-911.	1.5	88
59	First-principles calculation of spectral features, chemical shift and absolute threshold of ELNES and XANES using a plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104204.	0.7	88
60	Comparison of approximations in density functional theory calculations: Energetics and structure of binary oxides. Physical Review B, 2017, 96, .	1.1	85
61	Sparse representation for a potential energy surface. Physical Review B, 2014, 90, .	1.1	81
62	Calculation of multiplet structures ofCr3+andV3+inÎ±â^'Al2O3based on a hybrid method of density-functional theory and the configuration interaction. Physical Review B, 2000, 61, 143-161.	1.1	80
63	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. Journal of Chemical Physics, 2015, 143, 064710.	1.2	80
64	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. Physical Review B, 2008, 78, .	1.1	79
65	Theoretical ELNES using one-particle and multi-particle calculations. Micron, 2010, 41, 695-709.	1.1	79
66	Identification of ultradilute dopants in ceramics. Nature Materials, 2003, 2, 541-545.	13.3	78
67	First-Principles Study on Relaxor-Type Ferroelectric Behavior without Chemical Inhomogeneity in BaTaO₂N and SrTaO₂N. Chemistry of Materials, 2012, 24, 4343-4349.	3.2	78
68	Evolution of crystal structures in metallic elements. Physical Review B, 2013, 87, .	1.1	78
69	High-pressure torsion of titanium at cryogenic and room temperatures: Grain size effect on allotropic phase transformations. Acta Materialia, 2014, 68, 207-213.	3.8	78
70	Calculation of core-hole excitonic features on AlL23-edge x-ray-absorption spectra of Î±-Al2O3. Physical Review B, 1996, 54, 4604-4608.	1.1	75
71	Crystal structure, defect chemistry and oxygen ion transport of the ferroelectric perovskite, Na_{0.5}Bi_{0.5}TiO₃: insights from first-principles calculations. Journal of Materials Chemistry A, 2015, 3, 16574-16582.	5.2	72
72	New nanostructured phases with reversible hydrogen storage capability in immiscible magnesiumâ€“zirconium system produced by high-pressure torsion. Acta Materialia, 2016, 108, 293-303.	3.8	72

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73	First-principles interatomic potentials for ten elemental metals via compressed sensing. Physical Review B, 2015, 92, . Ionization potentials of (112) and (11<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10	1.1	71
74	of CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and CuGaSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><m	1.1	70
75	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. Entropy, 2018, 20, 655.	1.1	69
76	Atomic structures of supersaturated ZnOâ€“Al2O3 solid solutions. Journal of Applied Physics, 2008, 103, 014309.	1.1	68
77	Cubic and orthorhombic structures of aluminum hydrideAlH3predicted by a first-principles study. Physical Review B, 2005, 71, .	1.1	67
78	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. Physical Review B, 2006, 74, .	1.1	67
79	First-Principles Insight into the Hydration Ability and Proton Conduction of the Solid State Proton Conductor, Y and Sn Co-Doped BaZrO₃. Chemistry of Materials, 2015, 27, 901-908.	3.2	67
80	Electronic structure of indium oxide using cluster calculations. Physical Review B, 1997, 56, 3536-3539.	1.1	66
81	Electron Carrier Generation in a Refractory Oxide 12CaOÂ·7Al2O3by Heating in Reducing Atmosphere: Conversion from an Insulator to a Persistent Conductor. Journal of the American Ceramic Society, 2006, 89, 3294-3298.	1.9	65
82	Transition pathway of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>crystals under high pressures. Physical Review B, 2008, 77, .	1.1	65
83	Lattice thermal conductivities of two <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m polymorphs by first-principles calculations and the phonon Boltzmann transport equation. Physical Review B, 2018, 97, .	1.1	65
84	Ultra-severe plastic deformation: Evolution of microstructure, phase transformation and hardness in immiscible magnesium-based systems. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2017, 701, 158-166.	2.6	62
85	First-principles calculations of electron-energy-loss near-edge structure and near-edge x-ray-absorption fine structure of BN polytypes using model clusters. Physical Review B, 1999, 60, 4944-4951.	1.1	61
86	Doping of hexagonal boron nitride via intercalation: A theoretical prediction. Physical Review B, 2010, 81, .	1.1	61
87	Electronic and structural properties of the oxygen vacancy in BaTiO3. Applied Physics Letters, 2011, 98, .	1.5	61
88	Inversion Symmetry Breaking by Oxygen Octahedral Rotations in the Ruddlesden-Popper<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Na</mml:mi><mml:mi>R</mml:mi><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mr Physical Review Letters, 2014, 112, 187602.	2.9	60
89	Impurity-Enhanced Intergranular Cavity Formation in Silicon Nitride at High Temperatures. Journal of the American Ceramic Society, 1991, 74, 752-759.	1.9	59
90	Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation. Physical Review B, 2017, 95, .	1.1	59

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91	First-principles study of native defects and lanthanum impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>NaTaO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2003, 68, .	1.1	58
92	First-principles calculations of lattice dynamics in CdTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and CaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: Phase stability and ferroelectricity. Physical Review B, 2011, 84, .	1.1	58
93	Near-edge x-ray-absorption fine structure of crystalline silicon dioxides. Physical Review B, 1995, 52, 11733-11739.	1.1	56
94	Chemical bonding in titanium-metalloid compounds. Physical Review B, 1999, 59, 15033-15047.	1.1	56
95	First Principles Calculation of Fe L_{2,3}-edge X-ray Absorption Near Edge Structures of Iron Oxides. Materials Transactions, 2004, 45, 1414-1418.	0.4	56
96	Strategy for managing both high strength and large ductility in structural materialsâ€“sequential nucleation of different deformation modes based on a concept of plaston. Scripta Materialia, 2020, 181, 35-42.	2.6	55
97	Atomic structures and energetics ofLaNi5â^'Hsolid solution and hydrides. Physical Review B, 2001, 64, .	1.1	54
98	Crystal and Electronic Structure and Magnetic Properties of Divalent Europium Perovskite Oxides EuMO₃ (M = Ti, Zr, and Hf): Experimental and First-Principles Approaches. Inorganic Chemistry, 2012, 51, 4560-4567.	1.9	54
99	Ab initiostudy of symmetric tilt boundaries in ZnO. Physical Review B, 2001, 63, .	1.1	52
100	First principles study of dopant solubility and defect chemistry in LiCoO₂. Journal of Materials Chemistry A, 2014, 2, 11235-11245.	5.2	52
101	Firstâ€Principles Calculations of Anion Vacancies in Oxides and Nitrides. Journal of the American Ceramic Society, 2002, 85, 68-74.	1.9	51
102	Prediction of the new spinel phase ofTi3N4andSiTi2N4and the metal-insulator transition. Physical Review B, 2000, 61, 10609-10614.	1.1	50
103	Core-hole effect on dipolar and quadrupolar transitions ofSrTiO3andBaTiO3at TiKedge. Physical Review B, 2005, 71, .	1.1	50
104	First-principles multi-electron calculations for L2,3 ELNES/XANES of 3d transition metal monoxides. Ultramicroscopy, 2006, 106, 970-975.	0.8	50
105	Band offsets of CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/CdS and CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/ZnS (110) interfaces: A hybrid density functional theory study. Physical Review B, 2013, 88, .	1.1	50
106	First-Principles Calculations of Oxygen Vacancy Formation and Metallic Behavior at a Î²-MnO₂ Grain Boundary. ACS Applied Materials & Interfaces, 2015, 7, 1726-1734.	4.0	50
107	Electron energy loss near-edge structures of cubic Si3N4. Applied Physics Letters, 2001, 78, 2134-2136.	1.5	49
108	Local environment of Mn dopant in ZnO by near-edge x-ray absorption fine structure analysis. Applied Physics Letters, 2005, 86, 121902.	1.5	49

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109	Synthesis and electrochemistry of monoclinic Li(MnxFe1â^'x)BO3: a combined experimental and computational study. Journal of Materials Chemistry, 2011, 21, 10690.	6.7	49
110	Double thermoelectric power factor of a 2D electron system. Nature Communications, 2018, 9, 2224.	5.8	48
111	First-principles study of cation disordering inMgAl2O4spinel with cluster expansion and Monte Carlo simulation. Physical Review B, 2006, 73, .	1.1	47
112	Native defects in oxide semiconductors: a density functional approach. Journal of Physics Condensed Matter, 2010, 22, 384211.	0.7	47
113	Microstructure of Mn-doped Î³-Ga2O3 epitaxial film on sapphire (0001) with room temperature ferromagnetism. Journal of Applied Physics, 2007, 101, 063526.	1.1	46
114	Epitaxial growth of Mn-doped Î³-Ga₂O₃ on spinel substrate. Journal of Materials Research, 2011, 26, 578-583.	1.2	46
115	Defect chemistry of a BaZrO3 Î£3 (111) grain boundary by first principles calculations and spaceâ€“charge theory. Physical Chemistry Chemical Physics, 2012, 14, 12339.	1.3	46
116	Mode decomposition based on crystallographic symmetry in the band-unfolding method. Physical Review B, 2017, 95, .	1.1	46
117	Tuning the chemical functionality of a gas sensitive material: Water adsorption on SnO2(101). Surface Science, 2006, 600, 29-32.	0.8	45
118	Descriptors for Machine Learning of Materials Data. , 2018, , 3-23.		45
119	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953.	1.5	44
120	Conceptual and practical bases for the high accuracy of machine learning interatomic potentials: Application to elemental titanium. Physical Review Materials, 2017, 1, .	0.9	44
121	Atomic Structure of Luminescent Centers in High-Efficiency Ce-doped w-AlN Single Crystal. Scientific Reports, 2014, 4, 3778.	1.6	43
122	Categorization of surface polarity from a crystallographic approach. Computational Materials Science, 2016, 113, 221-230.	1.4	43
123	Changes in Chemical Bondings by Li Deintercalation in LiMO2(M=Cr, V, Co and Ni). Japanese Journal of Applied Physics, 1999, 38, 2024-2027.	0.8	42
124	First-principles calculation on free energy of precipitate nucleation. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2004, 28, 173-176.	0.7	42
125	Proton-Conducting Network in Lanthanum Orthophosphate. Journal of Physical Chemistry C, 2012, 116, 19117-19124.	1.5	42
126	Mn L2,3-edge X-ray absorption spectroscopic studies on charge-discharge mechanism of Li2MnO3. Applied Physics Letters, 2014, 104, .	1.5	42

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127	Theoretical prediction of ELNES/XANES and chemical bondings of AlN polytypes. Micron, 2003, 34, 249-254.	1.1	41
128	Strong Spinâ€Lattice Coupling Through Oxygen Octahedral Rotation in Divalent Europium Perovskites. Advanced Functional Materials, 2013, 23, 1864-1872.	7.8	41
129	Geometry and electronic structure of [0001]/(<ovl>1</ovl><ovl>2</ovl>30) Î£ = 7 symmetric tilt boundary in ZnO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2000, 80, 1567-1581.	0.8	40
130	First Principles Calculations of Formation Energies and Electronic Structures of Defects in Oxygen-Deficient LiMn[sub 2]O[sub 4]. Journal of the Electrochemical Society, 2003, 150, A63.	1.3	40
131	Distribution of solute atoms inÎ²- and spinelSi6âˆ'zAlzOzN8âˆ'zby AlK-edge x-ray absorption near-edge structure. Physical Review B, 2005, 71, .	1.1	40
132	Functional Complex Point-Defect Structure in a Huge-Size-Mismatch System. Physical Review Letters, 2013, 110, 065504.	2.9	40
133	Evaluation of Migration Energy of Lithium Ions in Chalcogenides and Halides by First Principles Calculation. Materials Transactions, 2002, 43, 1460-1463.	0.4	39
134	Theoretical Study on the Chemistry of Intergranular Glassy Film in Si₃N₄â€“SiO₂ Ceramics. Journal of the American Ceramic Society, 2002, 85, 109-112.	1.9	39
135	Thermal annealing effect on magnetism and cation distribution in disordered ZnFe2O4 thin films deposited on glass substrates. Journal of Magnetism and Magnetic Materials, 2007, 310, 2543-2545.	1.0	39
136	Theoretical Photovoltaic Conversion Efficiencies of ZnSnP₂, CdSnP₂, and Zn_{1-x}Cd_xSnP₂Alloys. Applied Physics Express, 2013, 6, 061201.	1.1	39
137	Oxygen Vacancy Formation and Reduction Properties of Î²-MnO₂ Grain Boundaries and the Potential for High Electrochemical Performance. ACS Applied Materials & Interfaces, 2014, 6, 17776-17784.	4.0	39
138	Matrix- and tensor-based recommender systems for the discovery of currently unknown inorganic compounds. Physical Review Materials, 2018, 2, .	0.9	39
139	Electron-energy-loss near edge structures of six-fold-coordinated Zn in MgO. Ultramicroscopy, 2001, 86, 363-370.	0.8	38
140	First Principles Calculation of Defect Formation Energies in Sr- and Mg-Doped LaGaO3. Journal of Physical Chemistry B, 2004, 108, 9168-9172.	1.2	38
141	Peak assignments of ELNES and XANES using overlap population diagrams. Ultramicroscopy, 2006, 106, 1120-1128.	0.8	38
142	Classification of spinel structures based on first-principles cluster expansion analysis. Physical Review B, 2010, 81, .	1.1	38
143	Electronic structures of dynamically stable As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	1.1	38
144	Effects of crystal structure on Co-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn> absorption near-edge structure and electron-energy-loss near-edge structure of trivalent cobalt oxides. Physical Review B, 2008, 77, .	1.1	37

#	Article	IF	Citations
145	Solubility of Si₃N₄ in Liquid SiO₂. Journal of the American Ceramic Society, 2002, 85, 25-32.	1.9	36
146	First-principles-based phase diagram of the cubic BNC ternary system. Physical Review B, 2008, 77, .	1.1	36
147	Phonon softening in paramagnetic bcc Fe and its relationship to the pressure-induced phase transition. Physical Review B, 2014, 90, .	1.1	36
148	Processing and Mechanical Properties of Dense Si3N4-SiC-Whisker Composites without Sintering Aids. Journal of the American Ceramic Society, 1989, 72, 1461-1464.	1.9	35
149	The study of Al-L23 ELNES with resolution-enhancement software and first-principles calculation. Journal of Electron Microscopy, 2003, 52, 299-303.	0.9	35
150	Theoretical Fingerprints of Transition Metal L_{2,3} XANES and ELNES for Lithium Transition Metal Oxides by ab Initio Multiplet Calculations. Journal of Physical Chemistry C, 2011, 115, 11871-11879.	1.5	34
151	Si3N4/SiC-Whisker Composites without Sintering Aids: III, High-Temperature Behavior. Journal of the American Ceramic Society, 1991, 74, 326-332.	1.9	33
152	Structures and energetics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Bi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> in a defective fluorite family derived by systematic first-principles lattice dynamics calculations. Physical Review B, 2010, 81, .	1.1	33
153	Compositional descriptor-based recommender system for the materials discovery. Journal of Chemical Physics, 2018, 148, 241719.	1.2	33
154	Effective Doping in Cubic Si₃N₄ and Ge₃N₄: A Firstâ€Principles Study. Journal of the American Ceramic Society, 2002, 85, 97-100.	1.9	32
155	Free-Energy Calculation of Precipitate Nucleation in an Fe-Cu-Ni Alloy. Materials Transactions, 2004, 45, 1978-1981.	0.4	32
156	First-principles study of the effect of lattice vibrations on Cu nucleation free energy in Fe-Cu alloys. Physical Review B, 2005, 72, .	1.1	32
157	First-principles calculations of the phase diagrams and band gaps in CuInSe2-CuGaSe2and CuInSe2-CuAlSe2pseudobinary systems. Physical Review B, 2012, 85, .	1.1	32
158	Proton trapping in Y and Sn Co-doped BaZrO₃. Journal of Materials Chemistry A, 2015, 3, 10045-10051.	5.2	32
159	Ordering and segregation of aCu75Pt25(111)surface: A first-principles cluster expansion study. Physical Review B, 2007, 76, .	1.1	31
160	Synthesis, crystal structure, and ionic conductivity of hydride ion-conducting Ln₂LiHO₃ (Ln = La, Pr, Nd) oxyhydrides. Journal of Materials Chemistry A, 2018, 6, 23457-23463.	5.2	31
161	Bulk nanocrystalline gamma magnesium hydride with low dehydrogenation temperature stabilized by plastic straining via high-pressure torsion. Scripta Materialia, 2018, 157, 54-57.	2.6	31
162	Group-theoretical high-order rotational invariants for structural representations: Application to linearized machine learning interatomic potential. Physical Review B, 2019, 99, .	1.1	31

#	Article	IF	Citations
163	Intrinsic fracture energy of polycrystalline silicon nitride. Philosophical Magazine Letters, 1993, 67, 95-100.	0.5	30
164	High-Temperature Strength of Fluorine-Doped Silicon Nitride. Journal of the American Ceramic Society, 1994, 77, 275-277.	1.9	30
165	First Principles Study on Factors Determining Battery Voltages of LiMO2(M=Ti-Ni). Japanese Journal of Applied Physics, 1999, 38, 4804-4808.	0.8	30
166	Atomic structures and bondings of Î²- and spinel-Si6â^'zAlzOzN8â^'zby first-principles calculations. Physical Review B, 2002, 66, .	1.1	30
167	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. Physical Review Materials, 2019, 3, .	0.9	30
168	Calculation of electron energy-loss near edge structures using a model cluster of MgO. Solid State Communications, 1995, 93, 533-536.	0.9	29
169	Theoretical calculation for the multiplet structure of the tetrahedrally coordinated Cr4+ in Y3Al5O12. Journal of Chemical Physics, 2001, 115, 492-508.	1.2	29
170	Theoretical Prediction of Postâ€Spinel Phases of Silicon Nitride. Journal of the American Ceramic Society, 2002, 85, 7-10.	1.9	29
171	First-principles calculations of x-ray absorption near edge structure and energy loss near edge structure: present and future. Journal of Physics Condensed Matter, 2009, 21, 104201.	0.7	29
172	Si3N4/SiC-Whisker Composites without Sintering Aids: II, Fracture Behavior. Journal of the American Ceramic Society, 1990, 73, 3039-3045.	1.9	28
173	Evaluation of Slow Crack Growth Resistance in Ceramics for High-Temperature Applications. Journal of the American Ceramic Society, 1992, 75, 772-777.	1.9	28
174	Improper Inversion Symmetry Breaking and Piezoelectricity through Oxygen Octahedral Rotations in Layered Perovskite Family, LiRTiO₄ (R = Rare Earths). Advanced Electronic Materials, 2016, 2, 1500196.	2.6	28
175	Low phonon conductivity of layered BiCuOS, BiCuOSe, and BiCuOTe from first principles. Physical Review B, 2016, 94, .	1.1	28
176	Tuning surface properties of SnO2(101) by reduction. Journal of Physics and Chemistry of Solids, 2006, 67, 1923-1929.	1.9	27
177	Effect of solute atoms on the chemical bonding of Fe₃C (cementite). The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1997, 75, 237-248.	0.6	26
178	Cluster calculation of oxygenK-edge electron-energy-loss near-edge structure of NiO. Physical Review B, 1998, 58, 9693-9696.	1.1	26
179	First-Principles Calculations of Migration Energy of Lithium Ions in Halides and Chalcogenides. Journal of Physical Chemistry B, 2006, 110, 8258-8262.	1.2	26
180	Hybrid density functional study of oxygen vacancies in KTaO3and NaTaO3. Physical Review B, 2011, 83, .	1.1	26

#	Article	IF	Citations
181	First-Principles Selection of Solute Elements for Er-Stabilized Bi₂O₃ Oxide-Ion Conductor with Improved Long-Term Stability at Moderate Temperatures. Chemistry of Materials, 2017, 29, 3763-3768.	3.2	26
182	Data-centric science for materials innovation. MRS Bulletin, 2018, 43, 659-663.	1.7	26
183	Electronic Structure and Defect Chemistry of Tin(II) Complex Oxide SnNb₂O₆. Journal of Physical Chemistry C, 2016, 120, 9604-9611.	1.5	25
184	Calculation of the Electronic Structure of sp Elements in beta-Si3N4 with Correlation to Solubility and Solution Effects. Journal of the American Ceramic Society, 1993, 76, 2833-2838.	1.9	24
185	Correlation between the electronic structure and hydrogen absorption characteristics in rare earth intermetallic compound hydrides. Journal of Alloys and Compounds, 1995, 221, 200-206.	2.8	24
186	Electronic States and Chemical Bondings of an Interstitial Cation in Ionic CompoundsAgCl and NaCl. Journal of the Physical Society of Japan, 1996, 65, 3582-3590.	0.7	24
187	First-principles molecular orbital calculation of electron energy-loss near-edge structures of -quartz. Journal Physics D: Applied Physics, 1996, 29, 1725-1729.	1.3	24
188	Valence state ofTiin conductive nanowires in sapphire. Physical Review B, 2004, 70, .	1.1	24
189	First-principles study of valence band offsets at ZnSnP2/CdS, ZnSnP2/ZnS, and related chalcopyrite/zincblende heterointerfaces. Journal of Applied Physics, 2013, 114, .	1.1	24
190	Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	24
191	Delayed-Failure Resistance of High-Purity Si3N4 at 1400oC. Journal of the American Ceramic Society, 1992, 75, 1023-1025.	1.9	23
192	Energetics and electronic structure of point defects associated with oxygen excess at a tilt boundary of ZnO. Journal of Materials Research, 2000, 15, 2167-2175.	1.2	23
193	Elastic constants and chemical bonding of LaNi5and LaNi5H7by first principles calculations. Journal of Physics Condensed Matter, 2003, 15, 6549-6561.	0.7	23
194	Interpretation of Siâ€L2,3 Edge Electron Energy Loss Near Edge Structures (ELNES) from Intergranular Glassy Film of Si3N4 Ceramics. Journal of the American Ceramic Society, 1999, 82, 3231-3236.	1.9	23
195	Local Chemical Bonding around Rareâ€Earth Ions in Î±â€and ÃŸâ€Si₃N₄. Journal of the American Ceramic Society, 1997, 80, 2525-2532.	1.9	23
196	Calculation of Grainâ€Boundary Bonding in Rareâ€Earthâ€Doped Î²â€Si₃N₄. Journal of the American Ceramic Society, 1998, 81, 565-570.	1.9	23
197	Co<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>K</mml:mi></mml:math>-edge XANES of LiCoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and CoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>with a variety of structures by supercell density f...	1.1	23
198	First principles study of thermal conductivity cross-over in nanostructured zinc-chalcogenides. Journal of Applied Physics, 2015, 117, .	1.1	23

#	Article	IF	Citations
199	Firstâ€principles study in an interâ€granular glassy film model of silicon nitride. Journal of the American Ceramic Society, 2018, 101, 2673-2688.	1.9	23
200	Electronic Mechanism of Ag-Cluster Formation in AgBr and AgI. Journal of the Physical Society of Japan, 1998, 67, 2027-2036.	0.7	22
201	Effect of Oxidation on Chemical Bonding around 3dTransition-Metal Impurities in ZnO. Japanese Journal of Applied Physics, 1999, 38, 3569-3575.	0.8	22
202	n- and p-type dopants for cubic silicon nitride. Applied Physics Letters, 2001, 78, 1577-1579.	1.5	22
203	Tetravalent Dysprosium in a Perovskiteâ€Type Oxide. Advanced Materials, 2012, 24, 2051-2053.	11.1	22
204	Thermoelectric phase diagram of the SrTiO3â€“SrNbO3 solid solution system. Journal of Applied Physics, 2017, 121, .	1.1	22
205	Competing Structural Instabilities in the Ruddlesdenâ€“Popper Derivatives HRTiO₄ (R = Rare) Tj ETQq1 1 0.784314 rgBT /O Centrosymmetricity. Chemistry of Materials, 2017, 29, 656-665.	3.2	22
206	Discovery of a Novel Sn(II)â€Based Oxide Î²â€SnMoO₄ for Daylightâ€Driven Photocatalysis. Advanced Science, 2017, 4, 1600246.	5.6	22
207	Densification and Microstructural Development of Silicon Nitride-Silica During Hot Isostatic Pressing. Journal of the American Ceramic Society, 1992, 75, 148-152.	1.9	21
208	Formation energy of Cr/Al vacancies in spinelMgCr2O4andMgAl2O4by first-principles calculations. Physical Review B, 2002, 65, .	1.1	21
209	Effect of local coordination of Mn on Mn-L2,3 edge electron energy loss spectrum. Journal of Applied Physics, 2013, 114, .	1.1	21
210	Variation of Zr-L_{2,3}XANES in tetravalent zirconium oxides. Journal of Physics Condensed Matter, 2013, 25, 165505.	0.7	21
211	First-Principles Calculations of Co Impurities and Native Defects in ZnO. Materials Transactions, 2002, 43, 1439-1443.	0.4	20
212	Theoretical Investigation of Al K-edge X-ray Absorption Spectra of Al, AlN and Al₂O₃. Materials Transactions, 2004, 45, 2031-2034.	0.4	20
213	Electronic Structures of Ln³⁺Î±â€SiAlONs with Correlations to Solubility and Solution Effects. Journal of the American Ceramic Society, 1996, 79, 2527-2532.	1.9	20
214	Proton incorporation and trapping in ZrO₂grain boundaries. Journal of Materials Chemistry A, 2014, 2, 1400-1408.	5.2	20
215	Ï‰ structure in steel: A first-principles study. Journal of Alloys and Compounds, 2016, 684, 624-627.	2.8	20
216	Linearized machine-learning interatomic potentials for non-magnetic elemental metals: Limitation of pairwise descriptors and trend of predictive power. Journal of Chemical Physics, 2018, 148, 234106.	1.2	20

#	Article	IF	Citations
217	Application of machine learning potentials to predict grain boundary properties in fcc elemental metals. Physical Review Materials, 2020, 4, .	0.9	20
218	High-Temperature Fracture Mechanism of Low-Ca-Doped Silicon Nitride. Journal of the American Ceramic Society, 1995, 78, 673-679.	1.9	19
219	Arsenic Removal by Hydroxyapatite-based Ceramics. Chemistry Letters, 2006, 35, 856-857.	0.7	19
220	Alkali-metal adsorption and manipulation on a hydroxylated TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(110) surface using atomic force microscopy. Physical Review B, 2011, 84, .	1.1	19
221	Local Structure and Energetics of Pr- and La-Doped SrTiO3 Grain Boundaries and the Influence on Coreâ€“Shell Structure Formation. Journal of Physical Chemistry C, 2014, 118, 25765-25778.	1.5	19
222	Li Intercalation into a Î²-MnO₂ Grain Boundary. ACS Applied Materials & Interfaces, 2015, 7, 8125-8131.	4.0	19
223	Temperature-dependent phonon spectra of magnetic random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	19
224	Fast material search of lithium ion conducting oxides using a recommender system. Journal of Materials Chemistry A, 2020, 8, 11582-11588.	5.2	19
225	High-Temperature Strength and Cavitation Threshold of Silicon Nitride-Silica Ceramics. Journal of the American Ceramic Society, 1992, 75, 195-200.	1.9	18
226	Site-specific electronic structure analysis by channeling EELS and first-principles calculations. Ultramicroscopy, 2006, 106, 1019-1023.	0.8	18
227	Grouping of structures for cluster expansion of multicomponent systems with controlled accuracy. Physical Review B, 2011, 83, .	1.1	18
228	Selective fabrication of nâ€•and pâ€type SnO films without doping. Physica Status Solidi - Rapid Research Letters, 2015, 9, 192-196.	1.2	18
229	Prediction of dielectric constants using a combination of first principles calculations and machine learning. Japanese Journal of Applied Physics, 2019, 58, SLLC01.	0.8	18
230	Si3N4/SiC-Whisker Composites without Sintering Aids: I, Quantitative Evaluation of Microstructure. Journal of the American Ceramic Society, 1990, 73, 3033-3038.	1.9	17
231	Calcia partition in phase-separated intergranular glass and interfaces in doped silicon nitride produced by hot isostatic pressing. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 422, 51-65.	2.6	17
232	Effects of Breit interaction on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:math> absorption near-edge structures of 3dtransition metals. Physical Review B, 2008, 77, .	1.1	17
233	Cluster expansion of multicomponent ionic systems with controlled accuracy: importance of long-range interactions in heterovalent ionic systems. Journal of Physics Condensed Matter, 2014, 26, 115403.	0.7	17
234	Stability of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï‰</mml:mi></mml:math>structure of transition elements. Physical Review B, 2016, 93, .	1.1	17

#	Article	IF	Citations
235	ciples thermodynamics of La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>-P<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	16
236	High temperature defect chemistry in layered lithium transition-metal oxides based on first-principles calculations. Journal of Power Sources, 2013, 244, 592-596.	4.0	16
237	Hot Isostatic Pressing and High-Temperature Strength of Silicon Nitride-Silica Ceramics. Journal of the American Ceramic Society, 1990, 73, 1095-1097.	1.9	15
238	Chemical bonding of transition metal disilicides. Intermetallics, 1996, 4, S113-S118.	1.8	15
239	Theoretical calculation for the multiplet structures of tetrahedrally coordinated Cr4+in silicate crystals. Journal of Physics Condensed Matter, 2001, 13, 5757-5784.	0.7	15
240	X-ray absorption near-edge structures of disordered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">Zn</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>solid solutions. Physical Review B, 2007, 76, .	1.1	15
241	Isostructural phase transitions of tetragonal perovskite titanates under negative hydrostatic pressure. Journal of Physics Condensed Matter, 2008, 20, 345207.	0.7	15
242	Atomic and electronic structures of the SrVO3-LaAlO3 interface. Journal of Applied Physics, 2011, 110, 046104.	1.1	15
243	Valence band offsets at zinc-blende heterointerfaces with misfit dislocations: A first-principles study. Physical Review B, 2013, 88, .	1.1	15
244	Protonic defects in yttria stabilized zirconia: incorporation, trapping and migration. Physical Chemistry Chemical Physics, 2014, 16, 4814.	1.3	15
245	Chemical bonding of3dtransition-metal disilicides. Physical Review B, 1998, 58, 9741-9745.	1.1	14
246	First-principles investigation of R2O3(ZnO)3 (R=Al, Ga, and In) in homologous series of compounds. Journal of Solid State Chemistry, 2008, 181, 137-142.	1.4	14
247	Site preference of cation vacancies in Mn-doped Ga2O3 with defective spinel structure. Applied Physics Letters, 2012, 101, .	1.5	14
248	First-principles molecular dynamics study for average structure and oxygen diffusivity at high temperature in cubic Bi₂O₃. Journal of Physics Condensed Matter, 2012, 24, 475402.	0.7	14
249	Nitrogen and hydrogen defect equilibria in Ca12Al14O33: a combined experimental and computational study. Journal of Materials Chemistry, 2012, 22, 15828.	6.7	14
250	Vibrational Effects in X-ray Absorption Spectra of Two-Dimensional Layered Materials. Journal of Physical Chemistry C, 2019, 123, 9688-9692.	1.5	14
251	Finite-displacement computation of the electron-phonon interaction within the projector augmented-wave method. Physical Review B, 2019, 100, .	1.1	14
252	Local geometries and energetics of hydrogen in acceptor-doped SrZrO3. Solid State Ionics, 2003, 162-163, 127-133.	1.3	13

#	Article	IF	Citations
253	Photocatalytic activity of Î±-PbO₂-type TiO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 822-826.	1.2	13
254	Atomistic structure and energetics of interface between Mn-doped Î³-Ga2O3 and MgAl2O4. Journal of Materials Science, 2011, 46, 4169-4175.	1.7	12
255	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. APL Materials, 2016, 4, 104809.	2.2	12
256	First-principles screening of structural properties of intermetallic compounds on martensitic transformation. Npj Computational Materials, 2017, 3, .	3.5	12
257	Valence Band Structure of ZnO (1010) Surface by Cluster Calculation. , 1999, 4, 69-80.		11
258	Energetics of Hydrogen States in SrZrO₃. Materials Transactions, 2002, 43, 1444-1450.	0.4	11
259	Lattice dynamics and thermal properties of SrHfO₃ by firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 1628-1633.	0.7	11
260	First-principles calculations of Znâ€“K XANES in Ca-deficient hydroxyapatite. Journal of Physics Condensed Matter, 2010, 22, 384213.	0.7	11
261	Efficient determination of alloy ground-state structures. Physical Review B, 2014, 90, .	1.1	11
262	Recommender System of Successful Processing Conditions for New Compounds Based on a Parallel Experimental Data Set. Chemistry of Materials, 2019, 31, 9984-9992.	3.2	11
263	Crystal Structures of the Cyclic Oligoesters from 6,8-Dioxabicyclo[3.2.1]octan-7-one. II. The Optically Inactive Cyclic Tetramer. Polymer Journal, 1982, 14, 197-203.	1.3	10
264	Positron Annihilation Study of Formation of Mg Vacancy in MgO. Materials Science Forum, 2004, 445-446, 153-155.	0.3	10
265	Magnetic properties of ilmenite-hematite solid-solution thin films: Direct observation of antiphase boundaries and their correlation with magnetism. Physical Review B, 2009, 80, .	1.1	10
266	Local environment of silicon in cubic boron nitride. Journal of Applied Physics, 2013, 114, 233502.	1.1	10
267	Impact of local strain on Ti-L_{2,3}electron energy-loss near-edge structures of BaTiO₃: a first-principles multiplet study. Microscopy (Oxford, England), 2014, 63, 249-254.	0.7	10
268	Materials informatics for dielectric materials. Japanese Journal of Applied Physics, 2018, 57, 11UB01.	0.8	10
269	First-Principles Study on the Stability of Weberite-Type, Pyrochlore, and Defect-Fluorite Structures of A₂³⁺B₂⁴⁺O₇ (A =) Tj ETQq1 1 0.784314 rgBT	1.5	10
270	Structure and Chemistry of Intergranular Films in Ca-Doped Si₃N₄. Materials Science Forum, 1996, 207-209, 729-732.	0.3	9

#	Article	IF	Citations
271	First-principles prediction of low-energy structures for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>AlH</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 79, .	1.1	9
272	Ab-initioCI calculations for 3dtransition metalL_{2,3}X-ray absorption spectra of TiCl₄and VOCl₃. Journal of Physics: Conference Series, 2009, 190, 012005.	0.3	9
273	Anisotropic phonon density of states in FePt nanoparticles withL10structure. Physical Review B, 2010, 81, .	1.1	9
274	Theoretical study on the structure and energetics of intergranular glassy film in Si₃N₄-SiO₂ceramics. International Journal of Materials Research, 2010, 101, 57-65.	0.1	9
275	Cluster expansion with controlled accuracy for the MgO/ZnO pseudobinary system via first-principles calculations. Physical Review B, 2012, 86, .	1.1	9
276	Significant Reduction in Hydration Energy for Yttria Stabilized Zirconia Grain Boundaries and the Consequences for Proton Conduction. Langmuir, 2014, 30, 10456-10464.	1.6	9
277	High Rate Performance of Dual-Substituted LiFePO₄ Based on Controlling Metastable Intermediate Phase. ACS Applied Energy Materials, 2018, 1, 6736-6740.	2.5	9
278	Six-fold coordinated silicon at grain boundaries in sintered Î±-Al2O3. Applied Physics Letters, 1998, 72, 191-193.	1.5	8
279	Prediction of the X-ray absorption near edge structure of the new high-density phase of SiO2. Physica Status Solidi (B): Basic Research, 2005, 242, R94-R96.	0.7	8
280	Beam damage suppression of low-Â porous Si-O-C films by cryo-electron-energy loss spectroscopy (EELS). Journal of Electron Microscopy, 2009, 58, 29-34.	0.9	8
281	Vanadium L2,3 XANES experiments and first-principles multielectron calculations: Impact of second-nearest neighboring cations on vanadium-bearing fresnoites. American Mineralogist, 2013, 98, 665-670.	0.9	8
282	Hot Isostatic Pressing of Synthesized Î²-Sialon Powders. Journal of the Ceramic Society of Japan, 1990, 98, 360-364.	1.3	7
283	The Role of Co Ions on the Appearance of Non-Linear I-V Characteristics of ZnO-Based Ceramics. Key Engineering Materials, 1999, 157-158, 249-256.	0.4	7
284	Multiplet structures of tetrahedrally coordinated Cr4+ and Cr5+ in Y3Al5O12. Applied Physics Letters, 2001, 78, 2154-2156.	1.5	7
285	First Principles Study of Core-hole Effect on Fluorine K-edge X-ray Absorption Spectra of MgF₂ and ZnF₂. Materials Transactions, 2004, 45, 1991-1993.	0.4	7
286	Inter-granular glassy phases in the low-CaO-doped HIPed Si₃N₄ceramics: a review. International Journal of Materials Research, 2010, 101, 66-74.	0.1	7
287	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. Journal of Materials Chemistry, 2010, 20, 10335.	6.7	7
288	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>A</mml:mi></mml:math> -site cation size effect on oxygen octahedral rotations in acentric Ruddlesden-Popper alkali rare-earth titanates. Physical Review Materials, 2019, 3, .	0.9	7

#	Article	IF	Citations
289	Electronic structure of 3d transition elements in Î²-Si₃N₄. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1995, 72, 459-473.	0.6	6
290	Theoretical calculation of oxygen K electron-energy-loss near-edge structures of Si-doped MgO. Journal of Physics Condensed Matter, 1999, 11, 5661-5670.	0.7	6
291	Calculation of Multiplet Structure of Ruby Using Explicit Effective Hamiltonian. Materials Transactions, JIM, 1999, 40, 396-399.	0.9	6
292	Electronic Structure and Chemical Bondings of MgCr2-xO4. Japanese Journal of Applied Physics, 2000, 39, 513-516.	0.8	6
293	First Principles Calculation of CO and H₂ Adsorption on Strained Pt Surface. Materials Transactions, 2008, 49, 2484-2490.	0.4	6
294	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. Physical Review B, 2009, 80, .	1.1	6
295	Atomic-level modeling and computation of intergranular glassy film in high-purity Si3N4 ceramics. Journal of the European Ceramic Society, 2012, 32, 1301-1311.	2.8	6
296	Stability of 12CaO·7Al₂O₃ Crystal under High-Pressure: Experimental and First-Principles Approaches. Materials Transactions, 2015, 56, 1350-1353.	0.4	6
297	Special quasirandom structure in heterovalent ionic systems. Physical Review B, 2015, 91, .	1.1	6
298	Equilibrium hydrogen pressures in the Vâ€“H system from first principles. International Journal of Hydrogen Energy, 2019, 44, 28909-28918.	3.8	6
299	Geometry and electronic structure of [0001]/(1 230) Î£ = 7 symmetric tilt boundary in ZnO. , 0, .		6
300	LO-mode phonon of KCl and NaCl at 300â€‰K by inelastic x-ray scattering measurements and first principles calculations. Journal of Physics Condensed Matter, 2022, 34, 365401.	0.7	6
301	Intergranular Glassy Films in Ceramics.. Journal of the Ceramic Society of Japan, 2001, 109, S127-S134.	1.3	5
302	Theoretical study of vibrational contribution on cluster formation in a binary alloy system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2004, 28, 167-171.	0.7	5
303	First-principles Calculation of L₃ X-ray Absorption Near Edge Structures (XANES) and Electron Energy Loss Near Edge Structures (ELNES) of GaN and InN Polymorphs. Materials Transactions, 2004, 45, 2023-2025.	0.4	5
304	First-principles study of defect-induced potentials in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ca</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2009, 80, .	1.1	5
305	All-electron CI calculations of 3d transition-metal L_{2,3}XANES using zeroth-order regular approximation for relativistic effects. Journal of Physics Condensed Matter, 2009, 21, 104209.	0.7	5
306	Epitaxial growth of tin(II) niobate with a pyrochlore structure. Journal of Crystal Growth, 2015, 416, 126-129.	0.7	5

#	Article	IF	Citations
307	First-principles calculations of high-pressure phase transition of TiO2 during decompression: From baddeleyite-type TiO2 to Î±-PbO2-type TiO2. Journal of Applied Physics, 2016, 120, 142108.	1.1	5
308	Analysis of Core-Hole Effect in Cation L2,3-Edge of MgO, Î±-Al2O3 and SiO2 Based on DV-XÎ± Cluster Calculations. Advances in Quantum Chemistry, 1998, , 441-466.	0.4	4
309	Theoretical Calculation for Multiplet Structure of Chromium Ion Pair in Ruby. Materials Transactions, JIM, 1999, 40, 416-419.	0.9	4
310	First principles calculations for modern ceramic science and engineering. Journal of Physics Condensed Matter, 2008, 20, 064215.	0.7	4
311	Process-Induced Damage Characterization of Patterned Low-Î° Film Using Electron Energy Loss Spectroscopy Technique. Japanese Journal of Applied Physics, 2010, 49, 111501.	0.8	4
312	Theoretical investigation of solid solution states of Ti1âˆ’V H2. Acta Materialia, 2017, 134, 274-282.	3.8	4
313	Solution effect on improved structural compatibility of NiTi-based alloys by systematic first-principles calculations. Journal of Applied Physics, 2019, 125, .	1.1	4
314	Local Chemical Bonding at Grain Boundary of Si3N4 Ceramics. , 1998, , 23-34.		4
315	Subcritical Crack Growth Resistance in Silicon Nitride Ceramics. , 1994, , 389-400.		4
316	First principles calculations of the formation energy of Cr/Al vacancies in spinel-type MgCr2O4 and MgAl2O4. International Journal of Quantum Chemistry, 2003, 91, 208-210.	1.0	3
317	Ground-state search in multicomponent magnetic systems. Physical Review B, 2012, 85, .	1.1	3
318	Combination of recommender system and single-particle diagnosis for accelerated discovery of novel nitrides. Journal of Chemical Physics, 2021, 154, 224117.	1.2	3
319	Cooperative Oxide-Ion Transport in Pyrochlore Y₂Ti₂O₇: A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry C, 2021, 125, 20460-20467.	1.5	3
320	HIPed Si3N4 for High Temperature Structural Applications at 1400Â°C. , 1992, , 73-78.		3
321	The Interaction between Vacancy and 3d-Transition Elements in Dilute Gold Alloys. Journal of the Physical Society of Japan, 1988, 57, 585-596.	0.7	2
322	Characterization of Grain Boundaries by Scanning Transmission Electron Microscopy.. Materia Japan, 1998, 37, 938-944.	0.1	2
323	Madelung energy of metalâ€“metalloid compounds. Computational Materials Science, 1999, 14, 62-66.	1.4	2
324	Electronic structures and electrode potentials of layered lithium insertion electrodes by the first principles calculation. Advances in Quantum Chemistry, 2003, 42, 145-161.	0.4	2

#	Article	IF	Citations
325	Surface design of alloy protection against CO-poisoning from first principles. Journal of Physics Condensed Matter, 2014, 26, 355006.	0.7	2
326	Phonon structure of titanium under shear deformation along <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>{</mml:mo><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover><mml:mn>2</mml:mn><mml:mo>}</mml:mo></mml:mro twinning mode. Physical Review B, 2020, 102, .	1.1	2
327	Data-Driven Materials Discovery from Large Chemistry Spaces. Matter, 2020, 3, 327-328.	5.0	2
328	Enumeration of nonequivalent substitutional structures using advanced data structure of binary decision diagram. Journal of Chemical Physics, 2020, 153, 104109.	1.2	2
329	Synthesisâ€condition recommender system discovers novel inorganic oxides. Journal of the American Ceramic Society, 0, , .	1.9	2
330	Proposing the Concept of Plaston and Strategy to Manage Both High Strength and Large Ductility in Advanced Structural Materials, on the Basis of Unique Mechanical Properties of Bulk Nanostructured Metals. , 2022, , 3-34.		2
331	Separation of the effects of charge transfer, covalency and electron correlations on the multiplet structure of ruby based on first-principles cluster calculations. Advances in Quantum Chemistry, 2000, 37, 69-83.	0.4	1
332	Atomic and Electronic Structure of Symmetric Tilt Boundaries in ZnO. Materials Research Society Symposia Proceedings, 2000, 654, 121.	0.1	1
333	Identification of Mg Vacancy in MgO by Positron Lifetime Measurements and First-Principles Calculations. Defect and Diffusion Forum, 2005, 242-244, 1-8.	0.4	1
334	Free Energy Calculations of Precipitate Nucleation. Materials Science Forum, 2007, 539-543, 2395-2400.	0.3	1
335	Phase relationships and structures of inorganic crystals by a combination of the cluster expansion method and first principles calculations. Journal of Physics Condensed Matter, 2010, 22, 384207.	0.7	1
336	Characterization of Si3N4/SiC Whisker Composites Without Additives: Analysis of Whisker Dispersion. Ceramic Engineering and Science Proceedings, 0, , 1015-1020.	0.1	1
337	Lifetime of HIPed Silicon Nitrides at Elevated Temperatures. , 1992, , 543-557.		1
338	Application of DV-Xα calculations in ceramics science. Advances in Quantum Chemistry, 2000, 37, 213-227.	0.4	0
339	ãƒªãƒ¦ãƒ¦ãƒ‰ãƒ³é›»æ±ºé‡åœæ–™è¨ˆ. Materia Japan, 2002, 41, 694-700.	0.1	0
340	FIRST-PRINCIPLES CALCULATION OF MULTIPLETS OF TRANSITION-METAL IONS IN CRYSTALS BASED ON DENSITY FUNCTIONAL METHOD. Recent Advances in Computational, 2002, , 278-292.	0.8	0
341	Electronic states associated with bond disorder at ZnO grain boundaries. Advances in Quantum Chemistry, 2003, 42, 175-186.	0.4	0
342	ç„¡æ©Ÿçµæ™¶ã,ã,ªãƒ³ä¼å°Žä½“ã®é‡åœæ–™è¨ˆ. Electrochemistry, 2007, 75, 421-425.	0.6	0

#	Article	IF	Citations
343	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. Key Engineering Materials, 2008, 403, 73-76.	0.4	0
344	First Principles Thermodynamics Calculations of Atomic Scale Modifications. Materia Japan, 2009, 48, 299-302.	0.1	0
345	First Principles Lattice Dynamics Calculations of Ag⁺ Doped KX (X=Cl, Br and I). Materials Transactions, 2009, 50, 999-1003.	0.4	0
346	Toward Materials Discovery with First-Principles Datasets and Learning Methods. Springer Series in Materials Science, 2016, , 173-186.	0.4	0
347	Materials Design Using First-Principles Calculations for Lithium-Ion Batteries. Materia Japan, 2017, 56, 430-433.	0.1	0
348	First-Principle Calculation of Peak Energies and Intensities in Optical Absorption Spectrum of Cr4+:Ca2GeO4. , 2000, , .		0
349	Theoretical Calculation of B-K ELNES(Electron Energy Loss Near Edge Structure) from 3d Transition Metal-Boron Systems. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2000, 64, 527-534.	0.2	0
350	The Lifetime of Silicon Nitride Limited by Cavity Nucleation in the Intergranular Glassy Phase. , 1992, , 209-218.		0
351	Properties of Silicon Nitride-Silica Ceramics Sintered by Hip. , 1992, , 79-84.		0
352	Complex Point Defect Structure in Cubic Boron Nitride. Materia Japan, 2016, 55, 609-609.	0.1	0
353	Recommender Systems for Materials Discovery. Lecture Notes in Physics, 2020, , 427-443.	0.3	0
354	Finding well-optimized special quasirandom structures with decision diagram. Physical Review Materials, 2021, 5, .	0.9	0