Zi-Jiang Liu

List of Publications by Year
in descending order

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142	2,217	257101	301761
papers	citations	24 h-index	39 g-index

142	142	142	2133
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	DFT and TDDFT study on organic dye sensitizers D5, DST and DSS for solar cells. Computational and Theoretical Chemistry, 2009, 899, 86-93.	1.5	137
2	DFT and TD-DFT study on structure and properties of organic dye sensitizer TA-St-CA. Current Applied Physics, 2010, 10, 77-83.	1.1	130
3	Orbital controlled band gap engineering of tetragonal BiFeO₃ for optoelectronic applications. Journal of Materials Chemistry C, 2018, 6, 1239-1247.	2.7	80
4	Optimizing the thermoelectric transport properties of Bi₂O₂Se monolayer via biaxial strain. Physical Chemistry Chemical Physics, 2019, 21, 15097-15105.	1.3	76
5	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO₃/SrTiO₃ Heterostructures. Nano Letters, 2015, 15, 4677-4684.	4.5	71
6	The Role of the Conjugate Bridge in Electronic Structures and Related Properties of Tetrahydroquinoline for Dye Sensitized Solar Cells. International Journal of Molecular Sciences, 2013, 14, 5461-5481.	1.8	66
7	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. Npj Computational Materials, 2021, 7, .	3.5	62
8	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. Nanomaterials, 2019, 9, 461.	1.9	60
9	A comparative study of low energy radiation responses of SiC, TiC and ZrC. Acta Materialia, 2016, 110, 192-199.	3.8	57
10	Understanding the Electronic Structures and Absorption Properties of Porphyrin Sensitizers YD2 and YD2-o-C8 for Dye-Sensitized Solar Cells. International Journal of Molecular Sciences, 2013, 14, 20171-20188.	1.8	54
11	Improved thermoelectric performance of bilayer Bi₂O₂Se by the band convergence approach. Journal of Materials Chemistry C, 2019, 7, 11029-11039.	2.7	53
12	A DFT study of mechanical properties, thermal conductivity and electronic structures of Th-doped Gd2Zr2O7. Acta Materialia, 2016, 121, 299-309.	3.8	48
13	Electronic structures and optical properties of organic dye sensitizer NKX derivatives for solar cells: A theoretical approach. Journal of Molecular Graphics and Modelling, 2012, 38, 419-429.	1.3	42
14	Heat capacity of ZnO with cubic structure at high temperatures. Solid State Communications, 2006, 140, 219-224.	0.9	35
15	A comparative study of the mechanical and thermal properties of defective ZrC, TiC and SiC. Scientific Reports, 2017, 7, 9344.	1.6	34
16	The phase transition, and elastic and thermodynamic properties of CaS derived from first-principles calculations. Journal of Physics Condensed Matter, 2008, 20, 115203.	0.7	33
17	Band Gap Reduction in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mo stretchy="false">(</mml:mo><mml:mi>Bi</mml:mi><mml:mi>Cr</mml:mi><mml:msub><mml:mrow><mml:mrow><mml:mi) Tj ETQq		

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19	Effects of doping Yb3+, La3+, Ti4+, Hf4+, Ce4+ cations on the mechanical properties, thermal conductivity, and electronic structures of Gd2Zr2O7. Journal of Alloys and Compounds, 2019, 776, 306-318.	2.8	30
20	Sound velocity measurements of tantalum under shock compression in the 10-110â€‰GPa range. Journal of Applied Physics, 2012, 111, 033511.	1.1	29
21	First-Principles Study of Point Defects in GaAs/AlAs Superlattice: the Phase Stability and the Effects on the Band Structure and Carrier Mobility. Nanoscale Research Letters, 2018, 13, 301.	3.1	29
22	Comparative study on electronic structures and optical properties of indoline and triphenylamine dye sensitizers for solar cells. Journal of Molecular Modeling, 2013, 19, 1553-1563.	0.8	27
23	Vacancy defects on optoelectronic properties of double perovskite Cs2AgBiBr6. Materials Science in Semiconductor Processing, 2021, 123, 105541.	1.9	27
24	Donor Halogenation Effects on Electronic Structures and Electron Process Rates of Donor/C₆₀ Heterojunction Interface: A Theoretical Study on F_nZnPc (n = 0, 4, 8, 16) and Cl_nSubPc (n = 0, 6). Journal of Physical Chemistry A, 2019, 123, 4034-4047.	1.1	26
25	The Electronic Structures and Optical Properties of Alkaline-Earth Metals Doped Anatase TiO2: A Comparative Study of Screened Hybrid Functional and Generalized Gradient Approximation. Materials, 2015, 8, 5508-5525.	1.3	25
26	A comparative study of low energy radiation response of AlAs, GaAs and GaAs/AlAs superlattice and the damage effects on their electronic structures. Scientific Reports, 2018, 8, 2012.	1.6	22
27	Theoretical investigations of the physical properties of tetragonal CaSiO3 perovskite. Solid State Communications, 2010, 150, 943-948.	0.9	21
28	Ab initio molecular dynamics simulation of the effects of stacking faults on the radiation response of 3C-SiC. Scientific Reports, 2016, 6, 20669.	1.6	21
29	Effects of Nd doping on the mechanical properties and electronic structures of Gd2Zr2O7: a first-principles-based study. Journal of Materials Science, 2018, 53, 16423-16438.	1.7	21
30	The Role of Porphyrin-Free-Base in the Electronic Structures and Related Properties of N-Fused Carbazole-Zinc Porphyrin Dye Sensitizers. International Journal of Molecular Sciences, 2015, 16, 27707-27720.	1.8	20
31	Thermal and mechanical stability, electronic structure and energetic properties of Pu-containing pyrochlores: La2-Pu Zr2O7 and La2Zr2-Pu O7 (0Ââ‰ÂyÂâ‰Â2). Journal of Nuclear Materials, 2015, 466, 162-171.	1.3	18
32	Fusing Thienyl with N-Annulated Perylene Dyes and Photovoltaic Parameters for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2020, 124, 3626-3635.	1.1	18
33	Electronic structures and absorption properties of three kinds of ruthenium dye sensitizers containing bipyridine-pyrazolate for solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1843-1848.	2.0	17
34	Molecular Docking toward Panchromatic Dye Sensitizers for Solar Cells Based upon Tetraazulenylporphyrin and Tetraanthracenylporphyrin. Journal of Physical Chemistry A, 2017, 121, 2655-2664.	1.1	17
35	Impact of isovalent and aliovalent substitution on the mechanical and thermal properties of Gd2Zr2O7. Scientific Reports, 2017, 7, 6399.	1.6	17
36	Structural stability and thermodynamic properties of BSb under high pressure and temperature. Materials Research Express, 2018, 5, 085904.	0.8	17

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37	Tunable characteristics of low-frequency bandgaps in two-dimensional multivibrator phononic crystal plates under prestrain. Scientific Reports, 2021, 11, 8389.	1.6	17
38	High pressure melting of MgO. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 353, 221-225.	0.9	16
39	Application of a shell model in molecular dynamics simulation to ZnO with zinc-blende cubic structure. Solid State Communications, 2007, 142, 15-19.	0.9	16
40	Tuning the electronic structures and related properties of Ruthenium-based dye sensitizers by ligands: A theoretical study and design. Computational and Theoretical Chemistry, 2013, 1017, 99-108.	1.1	15
41	Simulations on the wide bandgap characteristics of a two-dimensional tapered scatterer phononic crystal slab at low frequency. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126885.	0.9	15
42	The thermal and electrical transport properties of layered LaCuOSe under high pressure. Journal of Alloys and Compounds, 2021, 861, 157984.	2.8	15
43	Thermoelasticity of CaO from first principles. Chinese Physics B, 2007, 16, 499-505.	1.3	14
44	The electronic structures and optical properties of fullerene derivatives for organic solar cells: The number and size effects of fullerene-cage. Materials Chemistry and Physics, 2018, 204, 95-104.	2.0	14
45	Interface configuration effects on excitation, exciton dissociation, and charge recombination in organic photovoltaic heterojunction. International Journal of Quantum Chemistry, 2020, 120, e26103.	1.0	14
46	Electric field effects on organic photovoltaic heterojunction interfaces: The model case of pentacene/C60. Computational and Theoretical Chemistry, 2020, 1186, 112914.	1.1	14
47	Electronic, elastic and dynamic properties of the filled tetrahedral semiconductor LiMgN under pressures. Journal of Solid State Chemistry, 2015, 231, 1-6.	1.4	13
48	The electronic structures and excitation properties of three meso-pentafluorophenyl substituted zinc porphyrinâ€“fullerene dyad. Journal of Molecular Structure, 2018, 1173, 398-405.	1.8	13
49	A Theoretical Simulation of the Radiation Responses of Si, Ge, and Si/Ge Superlattice to Low-Energy Irradiation. Nanoscale Research Letters, 2018, 13, 133.	3.1	13
50	High-pressure and high-temperature physical properties of half-metallic full-Heusler alloy Mn 2 RuSi by first-principles and quasi-harmonic Debye model. Journal of Magnetism and Magnetic Materials, 2017, 424, 359-364.	1.0	13
51	The high-pressure melting curve of CaO. Solid State Communications, 2010, 150, 1785-1788.	0.9	12
52	The role of terminal groups in electronic structures and related properties: The case of pushâ€“pull porphyrin dye sensitizers for solar cells. Computational and Theoretical Chemistry, 2014, 1039, 62-70.	1.1	12
53	Enhancement of photocatalytic hydrogen evolution from dyeâ€“sensitized amideâ€“functionalized carbon nanospheres by superior adsorption performance. International Journal of Hydrogen Energy, 2020, 45, 30375-30386.	3.8	12
54	Fusion of thienyl into the backbone of electron acceptor in organic photovoltaic heterojunctions: a comparative study of BTPT-4F and BTPTT-4F. New Journal of Chemistry, 2020, 44, 5224-5234.	1.4	12

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55	Molecular dynamics study for the melting curve of MgO at high pressure. Chinese Physics B, 2004, 13, 384-387.	1.3	11
56	Thermal expansivity and bulk modulus of ZnO with NaCl-type cubic structure at high pressures and temperatures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 360, 362-366.	0.9	11
57	Molecular dynamics simulation of Pâ€“Vâ€“T relationship of ZnO with rock-salt structure using pair-wise interactions. Journal of Physics and Chemistry of Solids, 2007, 68, 249-255.	1.9	11
58	Shell and breathing shell model calculations for isothermal bulk modulus in MgO at high pressures and temperatures. Materials Chemistry and Physics, 2009, 116, 34-40.	2.0	11
59	Density functional calculations of the electronic structure and optical properties of magnesium oxide. Physica Status Solidi (B): Basic Research, 2010, 247, 157-162.	0.7	11
60	Elastic Tensor and Thermodynamic Property of Magnesium Silicate Perovskite from First-principles Calculations. Chinese Journal of Chemical Physics, 2011, 24, 703-710.	0.6	11
61	Molecular dynamics study on the structural and thermodynamic properties of the zinc-blende phase of GaN at high pressures and high temperatures. Wuli Xuebao/Acta Physica Sinica, 2005, 54, 5830.	0.2	11
62	Heat Capacity and Gruneisen Parameter for GaN with Zinc-Blende Structure. Chinese Journal of Chemical Physics, 2007, 20, 233-236.	0.6	10
63	Isothermal bulk modulus and its first pressure derivative of NaCl at high pressure and high temperature. Chinese Physics B, 2012, 21, 037103.	0.7	10
64	A comparative study of porphyrin dye sensitizers YD2-o-C8, SM315 and SM371 for solar cells: the electronic structures and excitation-related properties. European Physical Journal D, 2016, 70, 1.	0.6	10
65	Density functional theory study on the electronic structures and related properties of Ag-doped CH3NH3PbI3 perovskite. Results in Physics, 2019, 15, 102709.	2.0	10
66	Comparative study of the structural and thermodynamic properties of MgO at high pressures and high temperatures. Journal of Alloys and Compounds, 2008, 461, 279-284.	2.8	9
67	The melting curve of perovskite under lower mantle pressures. Solid State Communications, 2010, 150, 590-593.	0.9	9
68	The role of electronic donor moieties in porphyrin dye sensitizers for solar cells: Electronic structures and excitation related properties. Journal of Renewable and Sustainable Energy, 2017, 9, 053505.	0.8	9
69	Ab initio molecular dynamics simulation of the radiation damage effects of GaAs/AlGaAs superlattice. Journal of Nuclear Materials, 2019, 516, 228-237.	1.3	9
70	A comparative study of PffBT4T-2OD/EH-IDTBR and PffBT4T-2OD/PC71BM organic photovoltaic heterojunctions. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 412, 113225.	2.0	9
71	Application of shell model in molecular dynamics simulation to MgO. Chinese Physics B, 2004, 13, 1096-1099.	1.3	8
72	Thermoelasticity of MgO at High Pressures. Chinese Journal of Chemical Physics, 2007, 20, 65-70.	0.6	8

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73	Structural and thermodynamic properties of MgSiO3 perovskite under high pressure and high temperature. Solid State Communications, 2007, 144, 264-268.	0.9	8
74	Calculations of bond dissociation energies and dipole moments in energetic materials using density-functional methods. Journal of Hazardous Materials, 2007, 147, 658-662.	6.5	8
75	Elastic properties of the high-pressure rock-salt phase of ZnO. Philosophical Magazine Letters, 2008, 88, 181-190.	0.5	8
76	Simulated equation of state of CaF2 with fluorite-type structure at high temperature and high pressure. Physica B: Condensed Matter, 2009, 404, 158-162.	1.3	8
77	The low-frequency bandgap characteristics of a new three-dimensional multihole phononic crystal. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	8
78	The Halogenation Effects of Electron Acceptor ITIC for Organic Photovoltaic Nano-Heterojunctions. Nanomaterials, 2021, 11, 3417.	1.9	8
79	Simulation of Melting Behavior of the MgSiO3 Perovskite Under Lower Mantle Conditions. Chinese Journal of Chemical Physics, 2006, 19, 311-314.	0.6	7
80	First-principles study of the elastic and thermodynamic properties of CaSiO3perovskite. Journal of Physics Condensed Matter, 2007, 19, 246103.	0.7	7
81	High-pressure and high-temperature bulk modulus of cubic fluorite-type MgF2 from quasi-harmonic Debye model. Solid State Communications, 2011, 151, 1507-1510.	0.9	7
82	Molecular dynamics of NaCl melting under pressure. Physica B: Condensed Matter, 2012, 407, 60-63.	1.3	7
83	Electronic Structure, Phase Stability, and Elastic Properties of Inverse Heusler Compound Mn2RuSi at High Pressure. Journal of Superconductivity and Novel Magnetism, 2017, 30, 951-958.	0.8	7
84	High-pressure and high-temperature physical properties of LiF studied by density functional theory calculations and molecular dynamics simulations. Journal of Physics and Chemistry of Solids, 2018, 116, 209-215.	1.9	7
85	Assessment of Ab Initio and Density Functional Theory Methods for the Excitations of Donor-Acceptor Complexes: The Case of the Benzene-Tetracyanoethylene Model. International Journal of Molecular Sciences, 2018, 19, 1134.	1.8	7
86	Defect states and vibration energy recovery of novel two-dimensional piezoelectric phononic crystal plate. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 234206.	0.2	7
87	Comparative investigations of the Pâ€“Vâ€“T relationship of MgO with shell and breathing shell model molecular dynamics simulations. Physica B: Condensed Matter, 2007, 399, 9-16.	1.3	6
88	Comparative investigations of the thermal expansivity of MgO at high temperature. Materials Research Bulletin, 2009, 44, 1729-1733.	2.7	6
89	The electronic structure engineering of organic dye sensitizers for solar cells: The case of JK derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 855-866.	2.0	6
90	The bis-dimethylfluoreneaniline organic dye sensitizers for solar cells: A theoretical study and design. Journal of Molecular Graphics and Modelling, 2019, 88, 23-31.	1.3	6

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91	Effects of stacking periodicity on the electronic and optical properties of GaAs/AlAs superlattice: a first-principles study. Scientific Reports, 2020, 10, 4862.	1.6	6
92	Tunable low-frequency bandgaps of a new two-dimensional multi-component phononic crystal under different pressures, geometric parameters and pre-compression strains. Mechanics of Advanced Materials and Structures, 2022, 29, 4019-4031.	1.5	6
93	Simulated Melting Curve of NaCl up to 200 kbar. Chinese Physics Letters, 2003, 20, 2078-2080.	1.3	5
94	Calculations of the thermochemistry of six reactions leading to ammonia formation in Titan's atmosphere. Icarus, 2006, 183, 153-158.	1.1	5
95	Simulated Equations of State of MgSiO3 Perovskite. Chinese Journal of Chemical Physics, 2006, 19, 65-68.	0.6	5
96	Effect of pressure on the thermal expansion of MgO up to 200 GPa. Chinese Physics B, 2009, 18, 5001-5007.	0.7	5
97	The melting curve of MgSiO3perovskite from molecular dynamics simulation. Physica Scripta, 2011, 83, 045602.	1.2	5
98	STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF THE TETRAGONAL PHASE OFCaSiO₃PEROVSKITE UNDER PRESSURE: FIRST-PRINCIPLES CALCULATIONS. Modern Physics Letters B, 2011, 25, 41-52.	1.0	5
99	Molecular dynamic study of the melting temperature in MgF2 with the fluorite structure. Physica B: Condensed Matter, 2012, 407, 551-554.	1.3	5
100	First-principles prediction of the equation of state for TcC with rocksalt structure. Chemical Physics Letters, 2014, 614, 167-170.	1.2	5
101	Studying the phase transition, thermal expansion, and heat capacity of technetium mononitride by first-principles calculations. Chemical Physics Letters, 2016, 649, 64-67.	1.2	5
102	Density functional theory study of Î±-cyanoacrylic acid adsorbed on rutile TiO 2 (1 1 0) surface. Computational and Theoretical Chemistry, 2016, 1095, 125-133.	1.1	5
103	Thermal expansion, heat capacity and GrÃ¼neisen parameter of iridium phosphide Ir 2 P from quasi-harmonic Debye model. Solid State Communications, 2017, 253, 19-23.	0.9	5
104	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd2Zr2O7. Nanomaterials, 2019, 9, 196.	1.9	5
105	An AIMD+U simulation of low-energy displacement events in UO2. Journal of Nuclear Materials, 2020, 540, 152379.	1.3	5
106	A review of the properties, synthesis and applications of lanthanum copper oxychalcogenides. Journal Physics D: Applied Physics, 2022, 55, 273002.	1.3	5
107	Thermodynamic properties of magnesium oxide: a comparison ofab initioand empirical models. Physica Scripta, 2012, 85, 045702.	1.2	4
108	High-pressure physical properties of magnesium silicate post-perovskite from ab initio calculations. Bulletin of Materials Science, 2012, 35, 665-672.	0.8	4

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109	Optoelectronic properties of Rb-doped inorganic double perovskite Cs2AgBiBr6. Chemical Physics Letters, 2021, 771, 138501.	1.2	4
110	The mechanism of bandgap opening and merging in 2D spherical phononic crystals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 405, 127432.	0.9	4
111	Molecular dynamics of MgSiO 3 perovskite melting. Chinese Physics B, 2006, 15, 224-228.	1.3	3
112	Structure and thermal properties of the compound Li3AlB2O6. Journal of Physics Condensed Matter, 2006, 18, 6665-6675.	0.7	3
113	A revised additivity rule for electron scattering from ethylene, propene, butene, ethane, propane and butane. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 1535-1539.	0.6	3
114	Theoretical study on 2s2p⁶np Rydberg states of Cu¹⁹⁺ion. Chinese Physics B, 2012, 21, 013101.	0.7	3
115	Ab initio prediction of the first and second pressure derivatives of isothermal bulk modulus for the high-pressure rocksalt phase of ZnO. Chemical Physics Letters, 2013, 559, 46-49.	1.2	3
116	Electronic Structures and Optical Properties of Phenyl C71Butyric Acid Methyl Esters. Journal of Nanomaterials, 2013, 2013, 1-8.	1.5	3
117	Ab Initio Calculations of Structural, Electronic, and Mechanical Stability Properties of Magnesium Sulfide. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 403-410.	0.7	3
118	Phase stability, electronic structure and equation of state of cubic TcN from first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 3144-3148.	0.9	3
119	Optoelectronic properties of diathiafulvalene-functionalized diketopyrrolopyrroleâ€“fullerene molecular dyad. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118767.	2.0	3
120	Sol-gel processed tungsten trioxide nanocrystals layer for efficient hole-injection in quantum dot light-emitting diodes. Thin Solid Films, 2021, 730, 138722.	0.8	3
121	First-principles study of stability of point defects and their effects on electronic properties of GaAs/AlGaAs superlattice. Chinese Physics B, 2022, 31, 036104.	0.7	3
122	First-principles calculations of high-pressure physical properties anisotropy for magnesite. Scientific Reports, 2022, 12, 3691.	1.6	3
123	Density Functional Theory Study on Organic Dye Sensitizers Containing Bis-dimethylfluorenyl Amino Benzofuran. Chinese Journal of Chemical Physics, 2009, 22, 489-496.	0.6	2
124	Thermodynamic Properties of CaSiO₃ Perovskite at High Pressure and High Temperature. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 399-404.	0.7	2
125	The fine structure levels and spin-singlet contributions to zero-field-splitting parameters of Cr²⁺ion in CdGa₂S₄. Philosophical Magazine, 2010, 90, 1289-1295.	0.7	2
126	Effects of temperature and pressure on the thermal expansion of sodium chloride. Physica Scripta, 2012, 85, 045707.	1.2	2

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127	High-pressure phase transition and lattice dynamics of rock-salt and FeSi-type phases of MgS. Philosophical Magazine Letters, 2014, 94, 198-204.	0.5	2
128	Atomistic simulation of the structural and elastic properties of magnesite. Bulletin of Materials Science, 2016, 39, 1319-1325.	0.8	2
129	Development of the new interatomic potentials for the wurtzite phase of ZnO. Applied Physics A: Materials Science and Processing, 2022, 128, .	1.1	2
130	Total Cross-Sections for Electron Scattering of C3H6 Isomers: A Modified Additivity Rule Approach. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2007, 62, 716-720.	0.7	1
131	Calculation and evaluation of energy levels and radiative rates for and transitions in Cu XX. Atomic Data and Nuclear Data Tables, 2012, 98, 894-909.	0.9	1
132	The thermodynamic properties of cubic fluorite-type MgF₂: first-principles prediction. Physica Scripta, 2012, 85, 065707.	1.2	1
133	Molecular-dynamics simulations of hillocks induced by highly-charged Ar+, Xe+ ions impact on HOPG surface. Nuclear Instruments & Methods in Physics Research B, 2015, 362, 80-85.	0.6	1
134	Effects of temperature and energy on the radiation response of GaAs/AlAs and GaAs/AlGaAs superlattices. Radiation Physics and Chemistry, 2020, 174, 108983.	1.4	1
135	A Comparative Study of Electron Radiation Responses of Pu2Zr2O7 and La2Zr2O7: An abinitio Molecular Dynamics Study. Materials, 2021, 14, 1516.	1.3	1
136	Numerical prediction of structural stability and thermodynamic properties for MgF₂ with fluorite- type structure under high pressure. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 156202.	0.2	1
137	Effect of Sc, V, Zr, and Hf doping on the mechanical properties of TiB3 under high pressure. Applied Physics A: Materials Science and Processing, 2022, 128, 1.	1.1	1
138	THERMODYNAMIC PROPERTIES OF MgSiO₃ POST-PEROVSKITE. Modern Physics Letters B, 2010, 24, 315-324.	1.0	0
139	Inner-shell filling and X-ray emission of Ar¹⁷⁺ion in grazing incidence on an Al (111) surface. Canadian Journal of Physics, 2013, 91, 48-53.	0.4	0
140	Prediction on the high-pressure physical properties of a new metastable structure for BC₂N compound. Scientia Sinica: Physica, Mechanica Et Astronomica, 2019, 49, 078201.	0.2	0
141	Simulations of Formation of Nanostructure in Silicon Surface by Single Slow Highly Charged Ion. Journal of Physics: Conference Series, 2020, 1624, 022035.	0.3	0
142	Formamidinium dopant effects on double perovskite Cs 2 AgBiBr 6. International Journal of Quantum Chemistry, 2022, 122, e26846.	1.0	0