

# Zi-Jiang Liu

## List of Publications by Year in descending order

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Tunable low-frequency bandgaps of a new two-dimensional multi-component phononic crystal under different pressures, geometric parameters and pre-compression strains. <i>Mechanics of Advanced Materials and Structures</i> , 2022, 29, 4019-4031.	1.5	6
2	First-principles study of stability of point defects and their effects on electronic properties of GaAs/AlGaAs superlattice. <i>Chinese Physics B</i> , 2022, 31, 036104.	0.7	3
3	Formamidinium dopant effects on double perovskite Cs <sub>2</sub> AgBiBr <sub>6</sub> . <i>International Journal of Quantum Chemistry</i> , 2022, 122, e26846.	1.0	0
4	A review of the properties, synthesis and applications of lanthanum copper oxychalcogenides. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 273002.	1.3	5
5	Effect of Sc, V, Zr, and Hf doping on the mechanical properties of TiB <sub>3</sub> under high pressure. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, 1.	1.1	1
6	First-principles calculations of high-pressure physical properties anisotropy for magnesite. <i>Scientific Reports</i> , 2022, 12, 3691.	1.6	3
7	Development of the new interatomic potentials for the wurtzite phase of ZnO. <i>Applied Physics A: Materials Science and Processing</i> , 2022, 128, .	1.1	2
8	The thermal and electrical transport properties of layered LaCuOSe under high pressure. <i>Journal of Alloys and Compounds</i> , 2021, 861, 157984.	2.8	15
9	Vacancy defects on optoelectronic properties of double perovskite Cs <sub>2</sub> AgBiBr <sub>6</sub> . <i>Materials Science in Semiconductor Processing</i> , 2021, 123, 105541.	1.9	27
10	A Comparative Study of Electron Radiation Responses of Pu <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> and La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> : An abinitio Molecular Dynamics Study. <i>Materials</i> , 2021, 14, 1516.	1.3	1
11	Tunable characteristics of low-frequency bandgaps in two-dimensional multivibrator phononic crystal plates under prestrain. <i>Scientific Reports</i> , 2021, 11, 8389.	1.6	17
12	A comparative study of PffBT4T-2OD/EH-IDTBR and PffBT4T-2OD/PC71BM organic photovoltaic heterojunctions. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 412, 113225.	2.0	9
13	Optoelectronic properties of Rb-doped inorganic double perovskite Cs <sub>2</sub> AgBiBr <sub>6</sub> . <i>Chemical Physics Letters</i> , 2021, 771, 138501.	1.2	4
14	Sol-gel processed tungsten trioxide nanocrystals layer for efficient hole-injection in quantum dot light-emitting diodes. <i>Thin Solid Films</i> , 2021, 730, 138722.	0.8	3
15	The mechanism of bandgap opening and merging in 2D spherical phononic crystals. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 405, 127432.	0.9	4
16	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	62
17	The low-frequency bandgap characteristics of a new three-dimensional multihole phononic crystal. <i>Applied Physics A: Materials Science and Processing</i> , 2021, 127, 1.	1.1	8
18	The Halogenation Effects of Electron Acceptor ITIC for Organic Photovoltaic Nano-Heterojunctions. <i>Nanomaterials</i> , 2021, 11, 3417.	1.9	8

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19	Interface configuration effects on excitation, exciton dissociation, and charge recombination in organic photovoltaic heterojunction. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26103.	1.0	14
20	Simulations on the wide bandgap characteristics of a two-dimensional tapered scatterer phononic crystal slab at low frequency. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126885.	0.9	15
21	An AIMD+U simulation of low-energy displacement events in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2020, 540, 152379.	1.3	5
22	Electric field effects on organic photovoltaic heterojunction interfaces: The model case of pentacene/C60. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112914.	1.1	14
23	Enhancement of photocatalytic hydrogen evolution from dye-sensitized amide-functionalized carbon nanospheres by superior adsorption performance. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 30375-30386.	3.8	12
24	Optoelectronic properties of diathiafulvalene-functionalized diketopyrrolopyrrole-fullerene molecular dyad. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 242, 118767.	2.0	3
25	Effects of stacking periodicity on the electronic and optical properties of GaAs/AlAs superlattice: a first-principles study. <i>Scientific Reports</i> , 2020, 10, 4862.	1.6	6
26	Effects of temperature and energy on the radiation response of GaAs/AlAs and GaAs/AlGaAs superlattices. <i>Radiation Physics and Chemistry</i> , 2020, 174, 108983.	1.4	1
27	Fusion of thienyl into the backbone of electron acceptor in organic photovoltaic heterojunctions: a comparative study of BTPT-4F and BTPPT-4F. <i>New Journal of Chemistry</i> , 2020, 44, 5224-5234.	1.4	12
28	Fusing Thienyl with N-Annulated Perylene Dyes and Photovoltaic Parameters for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3626-3635.	1.1	18
29	Numerical prediction of structural stability and thermodynamic properties for MgF <sub>2</sub> with fluorite-type structure under high pressure. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020, 69, 156202.	0.2	1
30	Simulations of Formation of Nanostructure in Silicon Surface by Single Slow Highly Charged Ion. <i>Journal of Physics: Conference Series</i> , 2020, 1624, 022035.	0.3	0
31	Improved thermoelectric performance of bilayer Bi <sub>2</sub> O <sub>2</sub> Se by the band convergence approach. <i>Journal of Materials Chemistry C</i> , 2019, 7, 11029-11039.	2.7	53
32	Density functional theory study on the electronic structures and related properties of Ag-doped CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite. <i>Results in Physics</i> , 2019, 15, 102709.	2.0	10
33	Ab initio molecular dynamics simulation of the radiation damage effects of GaAs/AlGaAs superlattice. <i>Journal of Nuclear Materials</i> , 2019, 516, 228-237.	1.3	9
34	Optimizing the thermoelectric transport properties of Bi <sub>2</sub> O <sub>2</sub> Se monolayer via biaxial strain. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15097-15105.	1.3	76
35	Donor Halogenation Effects on Electronic Structures and Electron Process Rates of Donor/C <sub>60</sub> Heterojunction Interface: A Theoretical Study on F <sub>n</sub> ZnPc ( <i>n</i> = 0, 4, 8, 16) and Cl <sub>n</sub> SubPc ( <i>n</i> = 0, 6). <i>Journal of Physical Chemistry A</i> , 2019, 123, 4034-4047.	1.1	26
36	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. <i>Nanomaterials</i> , 2019, 9, 461.	1.9	60

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37	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . <i>Nanomaterials</i> , 2019, 9, 196.	1.9	5
38	The bis-dimethylfluoreneaniline organic dye sensitizers for solar cells: A theoretical study and design. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 88, 23-31.	1.3	6
39	Effects of doping Yb <sup>3+</sup> , La <sup>3+</sup> , Ti <sup>4+</sup> , Hf <sup>4+</sup> , Ce <sup>4+</sup> cations on the mechanical properties, thermal conductivity, and electronic structures of Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . <i>Journal of Alloys and Compounds</i> , 2019, 776, 306-318.	2.8	30
40	Prediction on the high-pressure physical properties of a new metastable structure for BC <sub>2</sub> N compound. <i>Scientia Sinica: Physica, Mechanica Et Astronomica</i> , 2019, 49, 078201.	0.2	0
41	Defect states and vibration energy recovery of novel two-dimensional piezoelectric phononic crystal plate. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2019, 68, 234206.	0.2	7
42	High-pressure and high-temperature physical properties of LiF studied by density functional theory calculations and molecular dynamics simulations. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 116, 209-215.	1.9	7
43	A comparative study of low energy radiation response of AlAs, GaAs and GaAs/AlAs superlattice and the damage effects on their electronic structures. <i>Scientific Reports</i> , 2018, 8, 2012.	1.6	22
44	Orbital controlled band gap engineering of tetragonal BiFeO <sub>3</sub> for optoelectronic applications. <i>Journal of Materials Chemistry C</i> , 2018, 6, 1239-1247.	2.7	80
45	The electronic structures and optical properties of fullerene derivatives for organic solar cells: The number and size effects of fullerene-cage. <i>Materials Chemistry and Physics</i> , 2018, 204, 95-104.	2.0	14
46	First-Principles Study of Point Defects in GaAs/AlAs Superlattice: the Phase Stability and the Effects on the Band Structure and Carrier Mobility. <i>Nanoscale Research Letters</i> , 2018, 13, 301.	3.1	29
47	Band-Gap Reduction in $\text{BiCrTjETQq}$		

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55	The role of electronic donor moieties in porphyrin dye sensitizers for solar cells: Electronic structures and excitation related properties. <i>Journal of Renewable and Sustainable Energy</i> , 2017, 9, 053505.	0.8	9
56	A comparative study of the mechanical and thermal properties of defective ZrC, TiC and SiC. <i>Scientific Reports</i> , 2017, 7, 9344.	1.6	34
57	Impact of isovalent and aliovalent substitution on the mechanical and thermal properties of Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . <i>Scientific Reports</i> , 2017, 7, 6399.	1.6	17
58	Electronic Structure, Phase Stability, and Elastic Properties of Inverse Heusler Compound Mn <sub>2</sub> RuSi at High Pressure. <i>Journal of Superconductivity and Novel Magnetism</i> , 2017, 30, 951-958.	0.8	7
59	High-pressure and high-temperature physical properties of half-metallic full-Heusler alloy Mn <sub>2</sub> RuSi by first-principles and quasi-harmonic Debye model. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 424, 359-364.	1.0	13
60	Ab initio molecular dynamics simulation of the effects of stacking faults on the radiation response of 3C-SiC. <i>Scientific Reports</i> , 2016, 6, 20669.	1.6	21
61	Studying the phase transition, thermal expansion, and heat capacity of technetium mononitride by first-principles calculations. <i>Chemical Physics Letters</i> , 2016, 649, 64-67.	1.2	5
62	A DFT study of mechanical properties, thermal conductivity and electronic structures of Th-doped Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . <i>Acta Materialia</i> , 2016, 121, 299-309.	3.8	48
63	Density functional theory study of $\hat{\pm}$ -cyanoacrylic acid adsorbed on rutile TiO <sub>2</sub> (1 1 0) surface. <i>Computational and Theoretical Chemistry</i> , 2016, 1095, 125-133.	1.1	5
64	Phase stability, electronic structure and equation of state of cubic TcN from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 3144-3148.	0.9	3
65	Atomistic simulation of the structural and elastic properties of magnesite. <i>Bulletin of Materials Science</i> , 2016, 39, 1319-1325.	0.8	2
66	A comparative study of porphyrin dye sensitizers YD2-o-C8, SM315 and SM371 for solar cells: the electronic structures and excitation-related properties. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	10
67	A comparative study of low energy radiation responses of SiC, TiC and ZrC. <i>Acta Materialia</i> , 2016, 110, 192-199.	3.8	57
68	The Role of Porphyrin-Free-Base in the Electronic Structures and Related Properties of N-Fused Carbazole-Zinc Porphyrin Dye Sensitizers. <i>International Journal of Molecular Sciences</i> , 2015, 16, 27707-27720.	1.8	20
69	The Electronic Structures and Optical Properties of Alkaline-Earth Metals Doped Anatase TiO <sub>2</sub> : A Comparative Study of Screened Hybrid Functional and Generalized Gradient Approximation. <i>Materials</i> , 2015, 8, 5508-5525.	1.3	25
70	Electronic, elastic and dynamic properties of the filled tetrahedral semiconductor LiMgN under pressures. <i>Journal of Solid State Chemistry</i> , 2015, 231, 1-6.	1.4	13
71	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO <sub>3</sub> /SrTiO <sub>3</sub> Heterostructures. <i>Nano Letters</i> , 2015, 15, 4677-4684.	4.5	71
72	The electronic structure engineering of organic dye sensitizers for solar cells: The case of JK derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 855-866.	2.0	6

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73	Thermal and mechanical stability, electronic structure and energetic properties of Pu-containing pyrochlores: La <sub>2</sub> -Pu Zr <sub>2</sub> O <sub>7</sub> and La <sub>2</sub> Zr <sub>2</sub> -Pu O <sub>7</sub> (O <sup>2-</sup> and Y <sup>3+</sup> ). Journal of Nuclear Materials, 2015, 466, 162-171.	1.3	18
74	Molecular-dynamics simulations of hillocks induced by highly-charged Ar <sup>+</sup> , Xe <sup>+</sup> ions impact on HOPG surface. Nuclear Instruments & Methods in Physics Research B, 2015, 362, 80-85.	0.6	1
75	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
76	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
77	First-principles prediction of the equation of state for TcC with rocksalt structure. Chemical Physics Letters, 2014, 614, 167-170.	1.2	5
78	The role of terminal groups in electronic structures and related properties: The case of push-pull porphyrin dye sensitizers for solar cells. Computational and Theoretical Chemistry, 2014, 1039, 62-70.	1.1	12
79	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
80	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
81	Inner-shell filling and X-ray emission of Ar <sup>17+</sup> ion in grazing incidence on an Al (111) surface. Canadian Journal of Physics, 2013, 91, 48-53.	0.4	0
82	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
83	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
84	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
85	Electronic Structures and Optical Properties of Phenyl C71Butyric Acid Methyl Esters. Journal of Nanomaterials, 2013, 2013, 1-8.	1.5	3
86	Sound velocity measurements of tantalum under shock compression in the 10-110 GPa range. Journal of Applied Physics, 2012, 111, 033511.	1.1	29
87	Effects of temperature and pressure on the thermal expansion of sodium chloride. Physica Scripta, 2012, 85, 045707.	1.2	2
88	Theoretical study on 2s2p <sup>6</sup> Rydberg states of Cu <sup>19+</sup> ion. Chinese Physics B, 2012, 21, 013101.	0.7	3
89	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
90	Thermodynamic properties of magnesium oxide: a comparison of ab initio and empirical models. Physica Scripta, 2012, 85, 045702.	1.2	4

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91	Electronic structures and optical properties of organic dye sensitizer NKX derivatives for solar cells: A theoretical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 419-429.	1.3	42
92	Calculation and evaluation of energy levels and radiative rates for and transitions in Cu XX. <i>Atomic Data and Nuclear Data Tables</i> , 2012, 98, 894-909.	0.9	1
93	High-pressure physical properties of magnesium silicate post-perovskite from ab initio calculations. <i>Bulletin of Materials Science</i> , 2012, 35, 665-672.	0.8	4
94	The thermodynamic properties of cubic fluorite-type MgF <sub>2</sub> : first-principles prediction. <i>Physica Scripta</i> , 2012, 85, 065707.	1.2	1
95	Molecular dynamics of NaCl melting under pressure. <i>Physica B: Condensed Matter</i> , 2012, 407, 60-63.	1.3	7
96	Molecular dynamic study of the melting temperature in MgF <sub>2</sub> with the fluorite structure. <i>Physica B: Condensed Matter</i> , 2012, 407, 551-554.	1.3	5
97	High-pressure and high-temperature bulk modulus of cubic fluorite-type MgF <sub>2</sub> from quasi-harmonic Debye model. <i>Solid State Communications</i> , 2011, 151, 1507-1510.	0.9	7
98	Electronic structures and absorption properties of three kinds of ruthenium dye sensitizers containing bipyridine-pyrazolate for solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1843-1848.	2.0	17
99	Elastic Tensor and Thermodynamic Property of Magnesium Silicate Perovskite from First-principles Calculations. <i>Chinese Journal of Chemical Physics</i> , 2011, 24, 703-710.	0.6	11
100	The melting curve of MgSiO <sub>3</sub> perovskite from molecular dynamics simulation. <i>Physica Scripta</i> , 2011, 83, 045602.	1.2	5
101	STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF THE TETRAGONAL PHASE OF CaSiO <sub>3</sub> PEROVSKITE UNDER PRESSURE: FIRST-PRINCIPLES CALCULATIONS. <i>Modern Physics Letters B</i> , 2011, 25, 41-52.	1.0	5
102	DFT and TD-DFT study on structure and properties of organic dye sensitizer TA-St-CA. <i>Current Applied Physics</i> , 2010, 10, 77-83.	1.1	130
103	A revised additivity rule for electron scattering from ethylene, propene, butene, ethane, propane and butane. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2010, 268, 1535-1539.	0.6	3
104	The melting curve of perovskite under lower mantle pressures. <i>Solid State Communications</i> , 2010, 150, 590-593.	0.9	9
105	Theoretical investigations of the physical properties of tetragonal CaSiO <sub>3</sub> perovskite. <i>Solid State Communications</i> , 2010, 150, 943-948.	0.9	21
106	The high-pressure melting curve of CaO. <i>Solid State Communications</i> , 2010, 150, 1785-1788.	0.9	12
107	Density functional calculations of the electronic structure and optical properties of magnesium oxide. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 157-162.	0.7	11
108	THERMODYNAMIC PROPERTIES OF MgSiO <sub>3</sub> POST-PEROVSKITE. <i>Modern Physics Letters B</i> , 2010, 24, 315-324.	1.0	0

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109	The fine structure levels and spin-singlet contributions to zero-field-splitting parameters of Cr <sup>2+</sup> ion in CdGa <sub>2</sub> S <sub>4</sub> . Philosophical Magazine, 2010, 90, 1289-1295.	0.7	2
110	Effect of pressure on the thermal expansion of MgO up to 200 GPa. Chinese Physics B, 2009, 18, 5001-5007.	0.7	5
111	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
112	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
113	Comparative investigations of the thermal expansivity of MgO at high temperature. Materials Research Bulletin, 2009, 44, 1729-1733.	2.7	6
114	Simulated equation of state of CaF <sub>2</sub> with fluorite-type structure at high temperature and high pressure. Physica B: Condensed Matter, 2009, 404, 158-162.	1.3	8
115	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
116	Thermodynamic Properties of CaSiO <sub>3</sub> Perovskite at High Pressure and High Temperature. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 399-404.	0.7	2
117	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
118	Elastic properties of the high-pressure rock-salt phase of ZnO. Philosophical Magazine Letters, 2008, 88, 181-190.	0.5	8
119	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
120	First-principles study of the elastic and thermodynamic properties of CaSiO <sub>3</sub> perovskite. Journal of Physics Condensed Matter, 2007, 19, 246103.	0.7	7
121	Heat Capacity and Gruneisen Parameter for GaN with Zinc-Blende Structure. Chinese Journal of Chemical Physics, 2007, 20, 233-236.	0.6	10
122	Thermoelasticity of MgO at High Pressures. Chinese Journal of Chemical Physics, 2007, 20, 65-70.	0.6	8
123	Thermoelasticity of CaO from first principles. Chinese Physics B, 2007, 16, 499-505.	1.3	14
124	Total Cross-Sections for Electron Scattering of C <sub>3</sub> H <sub>6</sub> Isomers: A Modified Additivity Rule Approach. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2007, 62, 716-720.	0.7	1
125	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
126	Structural and thermodynamic properties of MgSiO <sub>3</sub> perovskite under high pressure and high temperature. Solid State Communications, 2007, 144, 264-268.	0.9	8



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127	Comparative investigations of the P-V-T relationship of MgO with shell and breathing shell model molecular dynamics simulations. <i>Physica B: Condensed Matter</i> , 2007, 399, 9-16.	1.3	6
128	Molecular dynamics simulation of P-V-T relationship of ZnO with rock-salt structure using pair-wise interactions. <i>Journal of Physics and Chemistry of Solids</i> , 2007, 68, 249-255.	1.9	11
129	Calculations of bond dissociation energies and dipole moments in energetic materials using density-functional methods. <i>Journal of Hazardous Materials</i> , 2007, 147, 658-662.	6.5	8
130	Calculations of the thermochemistry of six reactions leading to ammonia formation in Titan's atmosphere. <i>Icarus</i> , 2006, 183, 153-158.	1.1	5
131	High pressure melting of MgO. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 353, 221-225.	0.9	16
132	Thermal expansivity and bulk modulus of ZnO with NaCl-type cubic structure at high pressures and temperatures. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2006, 360, 362-366.	0.9	11
133	First-principles calculation of elastic and thermodynamic properties of MgO and SrO under high pressure. <i>Physica B: Condensed Matter</i> , 2006, 373, 334-340.	1.3	32
134	Heat capacity of ZnO with cubic structure at high temperatures. <i>Solid State Communications</i> , 2006, 140, 219-224.	0.9	35
135	Molecular dynamics of MgSiO <sub>3</sub> perovskite melting. <i>Chinese Physics B</i> , 2006, 15, 224-228.	1.3	3
136	Structure and thermal properties of the compound Li <sub>3</sub> AlB <sub>2</sub> O <sub>6</sub> . <i>Journal of Physics Condensed Matter</i> , 2006, 18, 6665-6675.	0.7	3
137	Simulation of Melting Behavior of the MgSiO <sub>3</sub> Perovskite Under Lower Mantle Conditions. <i>Chinese Journal of Chemical Physics</i> , 2006, 19, 311-314.	0.6	7
138	Simulated Equations of State of MgSiO <sub>3</sub> Perovskite. <i>Chinese Journal of Chemical Physics</i> , 2006, 19, 65-68.	0.6	5
139	Molecular dynamics study on the structural and thermodynamic properties of the zinc-blende phase of GaN at high pressures and high temperatures. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2005, 54, 5830.	0.2	11
140	Application of shell model in molecular dynamics simulation to MgO. <i>Chinese Physics B</i> , 2004, 13, 1096-1099.	1.3	8
141	Molecular dynamics study for the melting curve of MgO at high pressure. <i>Chinese Physics B</i> , 2004, 13, 384-387.	1.3	11
142	Simulated Melting Curve of NaCl up to 200 kbar. <i>Chinese Physics Letters</i> , 2003, 20, 2078-2080.	1.3	5