Lijun Zhang

List of Publications by Year in Descending Order

158 papers	10,966 citations	52 h-index	102 g-index
169 ext. papers	13,613 ext. citations	10.1 avg, IF	6.6 L-index

#	Paper	IF	Citations
158	High-throughput computational material screening of the cycloalkane-based two-dimensional Dion–Jacobson halide perovskites for optoelectronics. *Chinese Physics B*, **2022**, 31, 037104	1.2	3
157	Global instability index as a crystallographic stability descriptor of halide and chalcogenide perovskites. *Journal of Energy Chemistry*, **2022**, 70, 1-8	12	2
156	Proton Transfer-Driven Modification of 3D Hybrid Perovskites to Form Oriented 2D Ruddlesden–Popper Phases. *Small Science*, **2022**, 2, 2100114		2
155	Radiative lifetimes, branching fractions, and oscillator strengths for highly excited levels in singly ionized tantalum (Ta ii). *Monthly Notices of the Royal Astronomical Society*, **2022**, 510, 4808-4818	4.3	
154	The Introduction of Defects in Ti 3 C 2 T x and Ti 3 C 2 T x -Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppb-Level NO 2 (Adv. Funct. Mater. 15/2022). *Advanced Functional Materials*, **2022**, 32, 2270091	15.6	0
153	Stability and electronic properties of two-dimensional metal–organic perovskites in Janus phase. *APL Materials*, **2021**, 9, 111105	5.7	1
152	Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications. *Journal of Physical Chemistry Letters*, **2021**, 12, 10532-10550	6.4	9
151	Controlled Synthesis of Pure-Phase GaAs Nanowires through Shear Tension. *ACS Photonics*, **2021**, 8, 2889-2897	6.5	0
150	Optical emission enhancement of bent InSe thin films. *Science China Information Sciences*, **2021**, 64, 1	3.4	2
149	Radiative parameters of high-lying levels in neutral rhodium. *Monthly Notices of the Royal Astronomical Society*, **2021**, 503, 5085-5090	4.3	1
148	Discovery of New Phases of Bismuth Oxyselenide Semiconductor Bi2OSe2 by Global Structure Search Approach. *Advanced Theory and Simulations*, **2021**, 4, 2000316	3.5	0
147	Electronic and optical properties of tapered tetrahedral semiconductor nanocrystals. *Nanotechnology*, **2021**, 32,	3.4	2
146	Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations. *Physical Review Materials*, **2021**, 5,	3.2	3
145	Alternative Lone-Pair ns -Cation-Based Semiconductors beyond Lead Halide Perovskites for Optoelectronic Applications. *Advanced Materials*, **2021**, 33, e2008574	24	9
144	Stable zero-dimensional cesium indium bromide hollow nanocrystals emitting blue light from self-trapped excitons. *Nano Today*, **2021**, 38, 101153	17.9	13
143	High-throughput computational materials screening and discovery of optoelectronic semiconductors. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11,	7.9	19
142	Band structure engineering through van der Waals heterostructing superlattices of two-dimensional transition metal dichalcogenides. *Informa Materia*, **2021**, 3, 201-211	23.1	13

141	High Color-Rendering Index and Stable White Light-Emitting Diodes by Assembling Two Broadband Emissive Self-Trapped Excitons. *Advanced Materials*, **2021**, 33, e2001367	24	74
140	Stable Cesium-Rich Formamidinium/Cesium Pure-Iodide Perovskites for Efficient Photovoltaics. *ACS Energy Letters*, **2021**, 6, 2735-2741	20.1	9
139	Molecular engineering towards efficientwhite-light-emitting perovskite. *Nature Communications*, **2021**, 12, 4890	17.4	10
138	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. *Science Bulletin*, **2021**, 66, 1973-1985	10.6	8
137	White Light-Emitting Diodes: High Color-Rendering Index and Stable White Light-Emitting Diodes by Assembling Two Broadband Emissive Self-Trapped Excitons (Adv. Mater. 2/2021). *Advanced Materials*, **2021**, 33, 2170010	24	2
136	Temperature-induced phase transition of two-dimensional semiconductor GaTe. *Chinese Physics B*, **2021**, 30, 016402	1.2	1
135	Rashba band splitting in two-dimensional Ruddlesden□Popper halide perovskites. *Journal of Applied Physics*, **2020**, 128, 175101	2.5	5
134	Discovery of New Polymorphs of Gallium Oxides with Particle Swarm Optimization-Based Structure Searches. *Advanced Electronic Materials*, **2020**, 6, 2000119	6.4	3
133	Observation of excitonic series in monolayer and few-layer black phosphorus. *Physical Review B*, **2020**, 101,	3.3	14
132	Enhanced Optical Emission from 2D InSe Bent onto Si-Pillars. *Advanced Optical Materials*, **2020**, 8, 2000828	8.1	10
131	Cd-Rich Alloyed CsPb Cd Br Perovskite Nanorods with Tunable Blue Emission and Fermi Levels Fabricated through Crystal Phase Engineering. *Advanced Science*, **2020**, 7, 2000930	13.6	28
130	New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties. *Advanced Functional Materials*, **2020**, 30, 2001920	15.6	19
129	Colloidal Synthesis of Ternary Copper Halide Nanocrystals for High-Efficiency Deep-Blue Light-Emitting Diodes with a Half-Lifetime above 100 h. *Nano Letters*, **2020**, 20, 3568-3576	11.5	121
128	Stable Yellow Light-Emitting Devices Based on Ternary Copper Halides with Broadband Emissive Self-Trapped Excitons. *ACS Nano*, **2020**, 14, 4475-4486	16.7	106
127	Proton-transfer-induced 3D/2D hybrid perovskites suppress ion migration and reduce luminance overshoot. *Nature Communications*, **2020**, 11, 3378	17.4	51
126	From Distortion to Disconnection: Linear Alkyl Diammonium Cations Tune Structure and Photoluminescence of Lead Bromide Perovskites. *Advanced Optical Materials*, **2020**, 8, 1902051	8.1	14
125	Computational functionality-driven design of semiconductors for optoelectronic applications. *Informa□□Materi□y*, **2020**, 2, 879-904	23.1	19
124	Imaging of the Atomic Structure of All-Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2020**, 11, 818-823	6.4	21

123	Halide Homogenization for High-Performance Blue Perovskite Electroluminescence. *Research*, **2020**, 2020, 9017871	7.8	20
122	Structural, Thermodynamical and Electronic Properties of All-Inorganic Lead Halide Perovskites. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2020**, 2007015-0	3.8	5
121	Van der Waals SnSe2(1−x)S2x Alloys: Composition-Dependent Bowing Coefficient and Electron–Phonon Interaction. *Advanced Functional Materials*, **2020**, 30, 1908092	15.6	10
120	Efficient and stable Ruddlesden–Popper perovskite solar cell with tailored interlayer molecular interaction. *Nature Photonics*, **2020**, 14, 154-163	33.9	251
119	Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains. *Physical Chemistry Chemical Physics*, **2020**, 22, 2122-2129	3.6	4
118	Bulk heterojunction gifts bismuth-based lead-free perovskite solar cells with record efficiency. *Nano Energy*, **2020**, 68, 104362	17.1	54
117	Electrically-Driven Violet Light-Emitting Devices Based on Highly Stable Lead-Free Perovskite Cs3Sb2Br9 Quantum Dots. *ACS Energy Letters*, **2020**, 5, 385-394	20.1	90
116	Color Tunable Self-Trapped Emissions from Lead-Free All Inorganic IA-IB Bimetallic Halides Cs-Ag-X (X = Cl, Br, I). *Small*, **2020**, 16, e2004272	11	18
115	Stabilizing Perovskite Solar Cells to IEC61215:2016 Standards with over 9,000-h Operational Tracking. *Joule*, **2020**, 4, 2646-2660	27.8	97
114	Stacking Effects on Electron-Phonon Coupling in Layered Hybrid Perovskites Microstrain Manipulation. *ACS Nano*, **2020**, 14, 5806-5817	16.7	24
113	Halogen Substitution in Zero-Dimensional Mixed Metal Halides toward Photoluminescence Modulation and Enhanced Quantum Yield. *Advanced Optical Materials*, **2020**, 8, 2000418	8.1	13
112	Extraordinary Temperature Dependent Second Harmonic Generation in Atomically Thin Layers of Transition-Metal Dichalcogenides. *Advanced Optical Materials*, **2020**, 8, 2000441	8.1	15
111	Spontaneous low-temperature crystallization of α-FAPbI3 for highly efficient perovskite solar cells. *Science Bulletin*, **2019**, 64, 1608-1616	10.6	27
110	Bottom-up growth of homogeneous Moiré superlattices in bismuth oxychloride spiral nanosheets. *Nature Communications*, **2019**, 10, 4472	17.4	31
109	Thermochromic Lead-Free Halide Double Perovskites. *Advanced Functional Materials*, **2019**, 29, 1807375	15.6	69
108	Solid salt confinement effect: An effective strategy to fabricate high crystalline polymer carbon nitride for enhanced photocatalytic hydrogen evolution. *Applied Catalysis B: Environmental*, **2019**, 246, 349-355	21.8	62
107	Ultrahigh-Performance Optoelectronics Demonstrated in Ultrathin Perovskite-Based Vertical Semiconductor Heterostructures. *ACS Nano*, **2019**, 13, 7996-8003	16.7	45
106	First-principles investigation of structural and electronic properties of oxygen adsorbing phosphorene. *Progress in Natural Science: Materials International*, **2019**, 29, 316-321	3.6	11

105	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. *ACS Applied Materials & Interfaces*, **2019**, 11, 24867-24875	9.5	7
104	Design of Mixed-Cation Tri-Layered Pb-Free Halide Perovskites for Optoelectronic Applications. *Advanced Electronic Materials*, **2019**, 5, 1900234	6.4	18
103	Ultrastable Lead-Free Double Perovskite Photodetectors with Imaging Capability. *Advanced Materials Interfaces*, **2019**, 6, 1900188	4.6	47
102	Switchable Out-of-Plane Polarization in 2D LiAlTe2. *Advanced Electronic Materials*, **2019**, 5, 1900089	6.4	13
101	Trifluoroacetate induced small-grained CsPbBr perovskite films result in efficient and stable light-emitting devices. *Nature Communications*, **2019**, 10, 665	17.4	227
100	Artificial control of in-plane anisotropic photoelectricity in monolayer MoS2. *Applied Materials Today*, **2019**, 15, 203-211	6.6	27
99	Zn-Alloyed CsPbI Nanocrystals for Highly Efficient Perovskite Light-Emitting Devices. *Nano Letters*, **2019**, 19, 1552-1559	11.5	256
98	Thermodynamically stabilized CsPbI-based perovskite solar cells with efficiencies >18. *Science*, **2019**, 365, 591-595	33.3	644
97	CsPb(I Br1)3 solar cells. *Science Bulletin*, **2019**, 64, 1532-1539	10.6	92
96	Ba-induced phase segregation and band gap reduction in mixed-halide inorganic perovskite solar cells. *Nature Communications*, **2019**, 10, 4686	17.4	65
95	Dopability of divalent tin containing phosphates for p-type transparent conductors. *Physical Review Materials*, **2019**, 3,	3.2	5
94	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. *Physical Review Materials*, **2019**, 3,	3.2	15
93	Atomically engineering activation sites onto metallic 1T-MoS catalysts for enhanced electrochemical hydrogen evolution. *Nature Communications*, **2019**, 10, 982	17.4	180
92	Strain engineering in perovskite solar cells and its impacts on carrier dynamics. *Nature Communications*, **2019**, 10, 815	17.4	286
91	Dimension Engineering of High-Quality InAs Nanostructures on a Wafer Scale. *Nano Letters*, **2019**, 19, 1632-1642	11.5	22
90	Ultrasensitive detection of miRNA with an antimonene-based surface plasmon resonance sensor. *Nature Communications*, **2019**, 10, 28	17.4	309
89	Two-Dimensional PC with Direct Band Gap and Anisotropic Carrier Mobility. *Journal of the American Chemical Society*, **2019**, 141, 1599-1605	16.4	76
88	InSe: a two-dimensional material with strong interlayer coupling. *Nanoscale*, **2018**, 10, 7991-7998	7.7	76

87	Chlorine-Incorporation-Induced Formation of the Layered Phase for Antimony-Based Lead-Free Perovskite Solar Cells. *Journal of the American Chemical Society*, **2018**, 140, 1019-1027	16.4	178
86	Formation and Diffusion of Metal Impurities in Perovskite Solar Cell Material CHNHPbI: Implications on Solar Cell Degradation and Choice of Electrode. *Advanced Science*, **2018**, 5, 1700662	13.6	82
85	Nanoporous Sulfur-Doped Copper Oxide (CuOS) for Overall Water Splitting. *ACS Applied Materials & Interfaces*, **2018**, 10, 745-752	9.5	59
84	Perovskite Photovoltaics: Pseudohalide-Induced Recrystallization Engineering for CH3NH3PbI3 Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells (Adv. Funct. Mater. 2/2018). *Advanced Functional Materials*, **2018**, 28, 1870013	15.6	5
83	Collective-Goldstone-mode-induced ultralow lattice thermal conductivity in Sn-filled skutterudite SnFe4Sb12. *Physical Review B*, **2018**, 97,	3.3	6
82	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. *Npj Computational Materials*, **2018**, 4,	10.9	55
81	Perovskite Solar Absorbers: Materials by Design. *Small Methods*, **2018**, 2, 1700316	12.8	78
80	Interlayer coupling in two-dimensional semiconductor materials. *Semiconductor Science and Technology*, **2018**, 33, 093001	1.8	23
79	Rational Design of Halide Double Perovskites for Optoelectronic Applications. *Joule*, **2018**, 2, 1662-1673	27.8	179
78	First-principle high-throughput calculations of carrier effective masses of two-dimensional transition metal dichalcogenides. *Journal of Semiconductors*, **2018**, 39, 072001	2.3	12
77	Rational design of new phases of tin monosulfide by first-principles structure searches. *Science China: Physics, Mechanics and Astronomy*, **2018**, 61, 1	3.6	11
76	Pb5Sb8S17 quantum dot-sensitized solar cells with an efficiency of 6% under 0.05 sun: Theoretical and experimental studies. *Progress in Photovoltaics: Research and Applications*, **2018**, 26, 205-213	6.8	6
75	Pseudohalide-Induced Recrystallization Engineering for CH3NH3PbI3 Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells. *Advanced Functional Materials*, **2018**, 28, 1704836	15.6	92
74	Rod-shaped thiocyanate-induced abnormal band gap broadening in SCN□doped CsPbBr3 perovskite nanocrystals. *Nano Research*, **2018**, 11, 2715-2723	10	30
73	Computational Design of Optoelectronic Semiconductor Materials **2018**,		1
72	Experimental Identification of Critical Condition for Drastically Enhancing Thermoelectric Power Factor of Two-Dimensional Layered Materials. *Nano Letters*, **2018**, 18, 7538-7545	11.5	50
71	Efficient and stable emission of warm-white light from lead-free halide double perovskites. *Nature*, **2018**, 563, 541-545	50.4	835
70	Dielectric Behavior as a Screen in Rational Searches for Electronic Materials: Metal Pnictide Sulfosalts. *Journal of the American Chemical Society*, **2018**, 140, 18058-18065	16.4	40

69	Robust Stability of Efficient Lead-Free Formamidinium Tin Iodide Perovskite Solar Cells Realized by Structural Regulation. *Journal of Physical Chemistry Letters*, **2018**, 9, 6999-7006	6.4	79
68	Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications. *Physical Review Applied*, **2018**, 10,	4.3	69
67	Pressure-induced emission of cesium lead halide perovskite nanocrystals. *Nature Communications*, **2018**, 9, 4506	17.4	134
66	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. *Journal of the American Chemical Society*, **2017**, 139, 2630-2638	16.4	490
65	Materials discovery at high pressures. *Nature Reviews Materials*, **2017**, 2,	73.3	266
64	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO(011) Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 7891-7896	9.5	22
63	Computer-Assisted Inverse Design of Inorganic Electrides. *Physical Review X*, **2017**, 7,	9.1	51
62	Cu-In Halide Perovskite Solar Absorbers. *Journal of the American Chemical Society*, **2017**, 139, 6718-6725	16.4	226
61	Highly Oriented Low-Dimensional Tin Halide Perovskites with Enhanced Stability and Photovoltaic Performance. *Journal of the American Chemical Society*, **2017**, 139, 6693-6699	16.4	558
60	Effects of manganese doping on the structure evolution of small-sized boron clusters. *Journal of Physics Condensed Matter*, **2017**, 29, 265401	1.8	14
59	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. *Journal of Applied Physics*, **2017**, 121, 225106	2.5	8
58	Construction of crystal structure prototype database: methods and applications. *Journal of Physics Condensed Matter*, **2017**, 29, 165901	1.8	17
57	Functionality-Directed Screening of Pb-Free Hybrid Organic□Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. *Chemistry of Materials*, **2017**, 29, 524-538	9.6	110
56	Discovery and ramifications of incidental Magn□ phase generation and release from industrial coal-burning. *Nature Communications*, **2017**, 8, 194	17.4	30
55	Doping Lanthanide into Perovskite Nanocrystals: Highly Improved and Expanded Optical Properties. *Nano Letters*, **2017**, 17, 8005-8011	11.5	447
54	Sn(II)-Containing Phosphates as Optoelectronic Materials. *Chemistry of Materials*, **2017**, 29, 2459-2465	9.6	16
53	New stable ternary alkaline-earth metal Pb(II) oxides: Ca/Sr/BaPb2O3 and BaPbO2. *Physical Review Materials*, **2017**, 1,	3.2	8
52	Intrinsic ultralow lattice thermal conductivity of the unfilled skutterudite FeSb3. *Physical Review B*, **2016**, 94,	3.3	18

51	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. *Physical Review Letters*, **2016**, 116, 057002	7.4	104
50	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH3NH3PbI3. *Chemistry of Materials*, **2016**, 28, 4349-4357	9.6	112
49	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. *Journal of Physical Chemistry Letters*, **2016**, 7, 597-602	6.4	72
48	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. *Chemistry of Materials*, **2016**, 28, 1746-1755	9.6	57
47	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications*, **2016**, 200, 87-95	4.2	29
46	CALYPSO structure prediction method and its wide application. *Computational Materials Science*, **2016**, 112, 406-415	3.2	102
45	Stability, electronic structures and thermoelectric properties of binary Zn$_3$Sb materials. *Journal of Materials Chemistry C*, **2016**, 4, 11305-11312	7.1	10
44	Design of ternary alkaline-earth metal Sn(II) oxides with potential good p-type conductivity. *Journal of Materials Chemistry C*, **2016**, 4, 4592-4599	7.1	23
43	Materials discovery via CALYPSO methodology. *Journal of Physics Condensed Matter*, **2015**, 27, 203203	1.8	63
42	Stabilization of fullerene-like boron cages by transition metal encapsulation. *Nanoscale*, **2015**, 7, 10482-9	7.7	59
41	Reinterpretation of the expected electronic density of states of semiconductor nanowires. *Nano Letters*, **2015**, 15, 88-95	11.5	8
40	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. *Scientific Reports*, **2015**, 5, 15433	4.9	56
39	Intrinsic Transparent Conductors without Doping. *Physical Review Letters*, **2015**, 115, 176602	7.4	26
38	N2H: a novel polymeric hydronitrogen as a high energy density material. *Journal of Materials Chemistry A*, **2015**, 3, 4188-4194	13	42
37	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. *APL Materials*, **2015**, 3, 011102	5.7	27
36	Evolution of electronic structure as a function of layer thickness in group-VIB transition metal dichalcogenides: emergence of localization prototypes. *Nano Letters*, **2015**, 15, 949-57	11.5	57
35	Genetic design of enhanced valley splitting towards a spin qubit in silicon. *Nature Communications*, **2013**, 4, 2396	17.4	32
34	The birth of a type-II nanostructure: carrier localization and optical properties of isoelectronically doped CdSe:Te nanocrystals. *ACS Nano*, **2012**, 6, 8325-34	16.7	14

33	Genomic design of strong direct-gap optical transition in Si/Ge core/multishell nanowires. *Nano Letters*, **2012**, 12, 984-91	11.5	43
32	Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. *Physical Review B*, **2011**, 84,	3.3	15
31	Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. *Physical Review B*, **2011**, 84,	3.3	10
30	Electronic structure of CsFe2Sb2 and its alloy with cobalt: A magnetic compound related to the iron superconductors. *Physical Review B*, **2010**, 81,	3.3	2
29	Electronic structure and thermoelectric properties: PbBi2Te4 and related intergrowth compounds. *Physical Review B*, **2010**, 81,	3.3	45
28	Electronic structure, localization, and spin-state transition in Cu-substituted FeSe:Fe1□CuxSe. *Physical Review B*, **2010**, 81,	3.3	38
27	Wide InP nanowires with wurtzite/zincblende superlattice segments are type-II whereas narrower nanowires become type-I: an atomistic pseudopotential calculation. *Nano Letters*, **2010**, 10, 4055-60	11.5	68
26	Zintl-phase compounds with SnSb4 tetrahedral anions: Electronic structure and thermoelectric properties. *Physical Review B*, **2010**, 81,	3.3	62
25	Density functional study of the overdoped iron chalcogenide TlFe2Se2 with ThCr2Si2 structure. *Physical Review B*, **2009**, 79,	3.3	35
24	Electronic structure and thermoelectric properties of layered PbSe-WSe2 materials. *Physical Review B*, **2009**, 80,	3.3	52
23	Electronic structure of Ba(Fe,Ru)2As2 and Sr(Fe,Ir)2As2 alloys. *Physical Review B*, **2009**, 79,	3.3	41
22	Density functional study of the electronic structure and magnetism of LaFeAsO alloyed with Zn. *Physical Review B*, **2009**, 80,	3.3	22
21	Electronic correlations in the iron pnictides. *Nature Physics*, **2009**, 5, 647-650	16.2	285
20	Density functional study of excess Fe in Fe1+xTe: Magnetism and doping. *Physical Review B*, **2009**, 79,	3.3	149
19	Electronic Structure, Magnetism and Spin-Fluctuations in Fe-As Based Superconductors. *Materials Research Society Symposia Proceedings*, **2008**, 1148, 1		
18	High-pressure phase transformations in CaH2. *Journal of Physics Condensed Matter*, **2008**, 20, 045211	1.8	20
17	Possible superconductivity in Fe-Sb based materials: Density functional study of LiFeSb. *Physical Review B*, **2008**, 78,	3.3	17
16	First-principles study of the pressure-induced rutile□CaCl2 phase transition in MgF2. *Solid State Communications*, **2008**, 145, 283-287	1.6	20

15	Electronic structures, lattice dynamics, and electron-phonon coupling of simple cubic Ca under pressure. *Solid State Communications*, **2008**, 146, 181-185	1.6	35
14	Density functional study of FeS, FeSe, and FeTe: Electronic structure, magnetism, phonons, and superconductivity. *Physical Review B*, **2008**, 78,	3.3	644
13	CaCl2-type high-pressure phase of magnesium hydride predicted by ab initio phonon calculations. *Physical Review B*, **2007**, 75,	3.3	33
12	First-principles study of the lattice dynamics, thermodynamic properties and electron-phonon coupling of YB6. *Physical Review B*, **2007**, 76,	3.3	39
11	Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study. *Physical Review B*, **2007**, 75,	3.3	37
10	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. *Solid State Communications*, **2007**, 141, 610-614	1.6	55
9	Pressure-induced enhancement of electron-phonon coupling in superconducting CaC6 from first principles. *Physical Review B*, **2006**, 74,	3.3	25
8	Phonon instabilities in rocksalt AgCl and AgBr under pressure studied within density functional theory. *Physical Review B*, **2006**, 74,	3.3	42
7	First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation. *Physical Review B*, **2005**, 72,	3.3	89
6	Pressure-Tailored Band Engineering for Significant Enhancements in the Photoelectric Performance of CsI3 in the Optical Communication Waveband. *Advanced Functional Materials*,2108636	15.6	5
5	Rational Design of Additive with Suitable Functional Groups Toward High-Quality FA 0.75 MA 0.25 SnI 3 Films and Solar Cells. *Solar Rrl*,2100800	7.1	1
4	Grain Boundaries in Methylammonium Lead Halide Perovskites Facilitate Water Diffusion. *Advanced Energy and Sustainability Research*,2100087	1.6	2
3	Evaluation of performance of machine learning methods in mining structure-property data of halide perovskite materials. *Chinese Physics B*,	1.2	2
2	The Introduction of Defects in Ti 3 C 2 T x and Ti 3 C 2 T x -Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppb-Level NO 2. *Advanced Functional Materials*,2108959	15.6	4
1	Entropy-Driven Stabilization of Multielement Halide Double-Perovskite Alloys. *Journal of Physical Chemistry Letters*,5017-5024	6.4	0