Lijun Zhang

List of Publications by Year
in descending order

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166 papers	16,383 citations	23567 58 h-index	15732 125 g-index
169 all docs	169 docs citations	169 times ranked	15920 citing authors

#	Article	IF	Citations
1	Pressureâ€Tailored Band Engineering for Significant Enhancements in the Photoelectric Performance of CsI₃ in the Optical Communication Waveband. Advanced Functional Materials, 2022, 32, 2108636.	14.9	18
2	Evaluation of performance of machine learning methods in mining structureâ€“property data of halide perovskite materials. Chinese Physics B, 2022, 31, 056302.	1.4	8
3	High-throughput computational material screening of the cycloalkane-based two-dimensional Dionâ€“Jacobson halide perovskites for optoelectronics. Chinese Physics B, 2022, 31, 037104.	1.4	8
4	Global instability index as a crystallographic stability descriptor of halide and chalcogenide perovskites. Journal of Energy Chemistry, 2022, 70, 1-8.	12.9	13
5	Proton Transferâ€Driven Modification of 3D Hybrid Perovskites to Form Oriented 2D Ruddlesdenâ€“Popper Phases. Small Science, 2022, 2, .	9.9	6
6	Radiative lifetimes, branching fractions, and oscillator strengths for highly excited levels in singly ionized tantalum (Ta <scp>ii</scp>). Monthly Notices of the Royal Astronomical Society, 2022, 510, 4808-4818.	4.4	0
7	The Introduction of Defects in Ti₃C₂T_x and Ti₃C₂T_xâ€Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppbâ€Level NO₂. Advanced Functional Materials, 2022, 32, .	14.9	21
8	The Introduction of Defects in Ti₃C₂T_x and Ti₃C₂T_xâ€Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppbâ€Level NO₂ (Adv. Funct. Mater. 15/2022). Advanced Functional Materials, 2022, 32, .	14.9	2
9	Thermal Shock Fabrication of Ionâ€Stabilized Perovskite and Solar Cells. Advanced Materials, 2022, 34, .	21.0	15
10	Two-dimensional Ruddlesden-Popper halide perovskite solar absorbers with short-chain interlayer spacers. Physical Review Materials, 2022, 6, .	2.4	5
11	Highâ€throughput computational materials screening and discovery of optoelectronic semiconductors. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	14.6	52
12	Band structure engineering through van der Waals heterostructing superlattices of <scp>twoâ€dimensional</scp> transition metal dichalcogenides. InformaÄnÃ-MateriÃ¡ly, 2021, 3, 201-211.	17.3	27
13	High Colorâ€Rendering Index and Stable White Lightâ€Emitting Diodes by Assembling Two Broadband Emissive Selfâ€Trapped Excitons. Advanced Materials, 2021, 33, e2001367.	21.0	162
14	Optical emission enhancement of bent InSe thin films. Science China Information Sciences, 2021, 64, 1.	4.3	6
15	Radiative parameters of high-lying levels in neutral rhodium. Monthly Notices of the Royal Astronomical Society, 2021, 503, 5085-5090.	4.4	2
16	Discovery of New Phases of Bismuth Oxyselenide Semiconductor Bi 2 OSe 2 by Global Structure Search Approach. Advanced Theory and Simulations, 2021, 4, 2000316.	2.8	2
17	Electronic and optical properties of tapered tetrahedral semiconductor nanocrystals. Nanotechnology, 2021, 32, 295203.	2.6	2
18	Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations. Physical Review Materials, 2021, 5, .	2.4	6

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19	Alternative Loneâ€Pair ns²â€Cationâ€Based Semiconductors beyond Lead Halide Perovskites for Optoelectronic Applications. Advanced Materials, 2021, 33, e2008574.	21.0	34
20	Helium incorporation induced direct-gap silicides. Npj Computational Materials, 2021, 7, .	8.7	6
21	Stable zero-dimensional cesium indium bromide hollow nanocrystals emitting blue light from self-trapped excitons. Nano Today, 2021, 38, 101153.	11.9	33
22	Stable Cesium-Rich Formamidinium/Cesium Pure-Iodide Perovskites for Efficient Photovoltaics. ACS Energy Letters, 2021, 6, 2735-2741.	17.4	31
23	Molecular engineering towards efficientwhite-light-emitting perovskite. Nature Communications, 2021, 12, 4890.	12.8	32
24	Grain Boundaries in Methylammonium Lead Halide Perovskites Facilitate Water Diffusion. Advanced Energy and Sustainability Research, 2021, 2, 2100087.	5.8	9
25	Heavy carrier effective masses in van der Waals semiconductor Sn(SeS) revealed by high magnetic fields up to 150 T. Physical Review B, 2021, 104, .	3.2	1
26	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. Science Bulletin, 2021, 66, 1973-1985.	9.0	32
27	White Lightâ€Emitting Diodes: High Colorâ€Rendering Index and Stable White Lightâ€Emitting Diodes by Assembling Two Broadband Emissive Selfâ€Trapped Excitons (Adv. Mater. 2/2021). Advanced Materials, 2021, 33, 2170010.	21.0	5
28	Temperature-induced phase transition of two-dimensional semiconductor GaTe*. Chinese Physics B, 2021, 30, 016402.	1.4	2
29	Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications. Journal of Physical Chemistry Letters, 2021, 12, 10532-10550.	4.6	20
30	Controlled Synthesis of Pure-Phase GaAs Nanowires through Shear Tension. ACS Photonics, 2021, 8, 2889-2897.	6.6	4
31	Stability and electronic properties of two-dimensional metalâ€“organic perovskites in Janus phase. APL Materials, 2021, 9, 111105.	5.1	2
32	Van der Waals SnSe 2(1â^' x) S 2 x Alloys: Compositionâ€Dependent Bowing Coefficient and Electronâ€“Phonon Interaction. Advanced Functional Materials, 2020, 30, 1908092.	14.9	18
33	Efficient and stable Ruddlesdenâ€“Popper perovskite solar cell with tailored interlayer molecular interaction. Nature Photonics, 2020, 14, 154-163.	31.4	443
34	Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains. Physical Chemistry Chemical Physics, 2020, 22, 2122-2129.	2.8	10
35	Bulk heterojunction gifts bismuth-based lead-free perovskite solar cells with record efficiency. Nano Energy, 2020, 68, 104362.	16.0	102
36	Electrically-Driven Violet Light-Emitting Devices Based on Highly Stable Lead-Free Perovskite Cs₃Sb₂Br₉ Quantum Dots. ACS Energy Letters, 2020, 5, 385-394.	17.4	169

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37	Color Tunable Selfâ€Trapped Emissions from Leadâ€Free All Inorganic IAâ€IB Bimetallic Halides Csâ€Agâ€X (X = Cl,) Tj ETQq1 1 0.784	10.0	44
38	Stabilizing Perovskite Solar Cells to IEC61215:2016 Standards with over 9,000-h Operational Tracking. Joule, 2020, 4, 2646-2660.	24.0	218
39	Rashba band splitting in two-dimensional Ruddlesdenâ€“Popper halide perovskites. Journal of Applied Physics, 2020, 128, 175101.	2.5	11
40	Discovery of New Polymorphs of Gallium Oxides with Particle Swarm Optimizationâ€Based Structure Searches. Advanced Electronic Materials, 2020, 6, 2000119.	5.1	17
41	Observation of excitonic series in monolayer and few-layer black phosphorus. Physical Review B, 2020, 101, .	3.2	25
42	Enhanced Optical Emission from 2D InSe Bent onto Siâ€Pillars. Advanced Optical Materials, 2020, 8, 2000828.	7.3	17
43	Cdâ€Rich Alloyed CsPb<sub>1â€_xCd_xBr₃ Perovskite Nanorods with Tunable Blue Emission and Fermi Levels Fabricated through Crystal Phase Engineering. Advanced Science, 2020, 7, 2000930.	11.2	52
44	Stable and luminescent halide perovskite fabricated in water. Light: Science and Applications, 2020, 9, 106.	16.6	18
45	New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties. Advanced Functional Materials, 2020, 30, 2001920.	14.9	33
46	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.	9.1	200
47	Stable Yellow Light-Emitting Devices Based on Ternary Copper Halides with Broadband Emissive Self-Trapped Excitons. ACS Nano, 2020, 14, 4475-4486.	14.6	199
48	Proton-transfer-induced 3D/2D hybrid perovskites suppress ion migration and reduce luminance overshoot. Nature Communications, 2020, 11, 3378.	12.8	108
49	From Distortion to Disconnection: Linear Alkyl Diammonium Cations Tune Structure and Photoluminescence of Lead Bromide Perovskites. Advanced Optical Materials, 2020, 8, 1902051.	7.3	30
50	Computational functionalityâ€driven design of semiconductors for optoelectronic applications. InformaÄnÃ-MateriÃ¡ly, 2020, 2, 879-904.	17.3	32
51	Imaging of the Atomic Structure of All-Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 818-823.	4.6	26
52	Stacking Effects on Electronâ€“Phonon Coupling in Layered Hybrid Perovskites via Microstrain Manipulation. ACS Nano, 2020, 14, 5806-5817.	14.6	50
53	Halogen Substitution in Zeroâ€Dimensional Mixed Metal Halides toward Photoluminescence Modulation and Enhanced Quantum Yield. Advanced Optical Materials, 2020, 8, 2000418.	7.3	29
54	Extraordinary Temperature Dependent Second Harmonic Generation in Atomically Thin Layers of Transitionâ€Metal Dichalcogenides. Advanced Optical Materials, 2020, 8, 2000441.	7.3	30

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55	Halide Homogenization for High-Performance Blue Perovskite Electroluminescence. Research, 2020, 2020, 9017871.	5.7	32
56	Structural, Thermodynamical and Electronic Properties of All-Inorganic Lead Halide Perovskites. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2020, .	4.9	9
57	Thermodynamically stabilized Î²-CsPbI ₃ â€“based perovskite solar cells with efficiencies >18%. Science, 2019, 365, 591-595.	12.6	963
58	CsPb(I Br1â^')3 solar cells. Science Bulletin, 2019, 64, 1532-1539.	9.0	114
59	Ba-induced phase segregation and band gap reduction in mixed-halide inorganic perovskite solar cells. Nature Communications, 2019, 10, 4686.	12.8	105
60	Spontaneous low-temperature crystallization of Î±-FAPbI3 for highly efficient perovskite solar cells. Science Bulletin, 2019, 64, 1608-1616.	9.0	58
61	Bottom-up growth of homogeneous MoirÃ© superlattices in bismuth oxychloride spiral nanosheets. Nature Communications, 2019, 10, 4472.	12.8	59
62	Thermochromic Leadâ€Free Halide Double Perovskites. Advanced Functional Materials, 2019, 29, 1807375.	14.9	120
63	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.	20.2	136
64	Ultrahigh-Performance Optoelectronics Demonstrated in Ultrathin Perovskite-Based Vertical Semiconductor Heterostructures. ACS Nano, 2019, 13, 7996-8003.	14.6	64
65	Preface to the Special Issue on 2D-Materials-Related Physical Properties and Optoelectronic Devices. Journal of Semiconductors, 2019, 40, 060101.	3.7	4
66	First-principles investigation of structural and electronic properties of oxygen adsorbing phosphorene. Progress in Natural Science: Materials International, 2019, 29, 316-321.	4.4	12
67	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. ACS Applied Materials & Interfaces, 2019, 11, 24867-24875.	8.0	11
68	Design of Mixedâ€Cation Triâ€Layered Pbâ€Free Halide Perovskites for Optoelectronic Applications. Advanced Electronic Materials, 2019, 5, 1900234.	5.1	21
69	Ultrastable Leadâ€Free Double Perovskite Photodetectors with Imaging Capability. Advanced Materials Interfaces, 2019, 6, 1900188.	3.7	62
70	Switchable Outâ€ofâ€Plane Polarization in 2D LiAlTe₂. Advanced Electronic Materials, 2019, 5, 1900089.	5.1	20
71	Trifluoroacetate induced small-grained CsPbBr3 perovskite films result in efficient and stable light-emitting devices. Nature Communications, 2019, 10, 665.	12.8	350
72	Artificial control of in-plane anisotropic photoelectricity in monolayer MoS2. Applied Materials Today, 2019, 15, 203-211.	4.3	45

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73	Zn-Alloyed CsPbI₃ Nanocrystals for Highly Efficient Perovskite Light-Emitting Devices. Nano Letters, 2019, 19, 1552-1559.	9.1	395
74	Atomically engineering activation sites onto metallic 1T-MoS2 catalysts for enhanced electrochemical hydrogen evolution. Nature Communications, 2019, 10, 982.	12.8	311
75	Strain engineering in perovskite solar cells and its impacts on carrier dynamics. Nature Communications, 2019, 10, 815.	12.8	528
76	Dimension Engineering of High-Quality InAs Nanostructures on a Wafer Scale. Nano Letters, 2019, 19, 1632-1642.	9.1	29
77	Ultrasensitive detection of miRNA with an antimonene-based surface plasmon resonance sensor. Nature Communications, 2019, 10, 28.	12.8	475
78	Two-Dimensional PC₆ with Direct Band Gap and Anisotropic Carrier Mobility. Journal of the American Chemical Society, 2019, 141, 1599-1605.	13.7	144
79	Dopability of divalent tin containing phosphates for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type transparent conductors. Physical Review Materials, 2019, 3, .	2.4	5
80	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	2.4	20
81	Thermochromic Lead-free Halide Double Perovskites. , 2019, , .		0
82	InSe: a two-dimensional material with strong interlayer coupling. Nanoscale, 2018, 10, 7991-7998.	5.6	102
83	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.	13.7	241
84	Formation and Diffusion of Metal Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃: Implications on Solar Cell Degradation and Choice of Electrode. Advanced Science, 2018, 5, 1700662.	11.2	130
85	Nanoporous Sulfur-Doped Copper Oxide (Cu₂O_xS_{1â€“x}) for Overall Water Splitting. ACS Applied Materials & Interfaces, 2018, 10, 745-752.	8.0	83
86	Perovskite Photovoltaics: Pseudohalideâ€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.	14.9	5
87	Collective-Goldstone-mode-induced ultralow lattice thermal conductivity in Sn-filled skutterudite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SnFe</mml:mi><mml:mn>4</mml:mn></ Physical Review B, 2018, 97, .	3.2	11
88	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. Npj Computational Materials, 2018, 4, .	8.7	86
89	Perovskite Solar Absorbers: Materials by Design. Small Methods, 2018, 2, 1700316.	8.6	95
90	<scp>Pb₅Sb₈S₁₇</scp> quantum dotâ€sensitized solar cells with an efficiency of 6% under 0.05 sun: <scp>T</scp>heoretical and experimental studies. Progress in Photovoltaics: Research and Applications, 2018, 26, 205-213.	8.1	13

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91	Pseudohalideâ€Induced Recrystallization Engineering for CH₃NH₃PbI₃ Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells. Advanced Functional Materials, 2018, 28, 1704836.	14.9	112
92	Rod-shaped thiocyanate-induced abnormal band gap broadening in SCNâ^' doped CsPbBr3 perovskite nanocrystals. Nano Research, 2018, 11, 2715-2723.	10.4	44
93	Computational Design of Optoelectronic Semiconductor Materials. , 2018, , .		1
94	Experimental Identification of Critical Condition for Drastically Enhancing Thermoelectric Power Factor of Two-Dimensional Layered Materials. Nano Letters, 2018, 18, 7538-7545.	9.1	72
95	Efficient and stable emission of warm-white light from lead-free halide double perovskites. Nature, 2018, 563, 541-545.	27.8	1,451
96	Dielectric Behavior as a Screen in Rational Searches for Electronic Materials: Metal Pnictide Sulfosalts. Journal of the American Chemical Society, 2018, 140, 18058-18065.	13.7	69
97	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.	4.6	117
98	Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications. Physical Review Applied, 2018, 10, .	3.8	109
99	Pressure-induced emission of cesium lead halide perovskite nanocrystals. Nature Communications, 2018, 9, 4506.	12.8	212
100	Interlayer coupling in two-dimensional semiconductor materials. Semiconductor Science and Technology, 2018, 33, 093001.	2.0	29
101	Rational Design of Halide Double Perovskites for Optoelectronic Applications. Joule, 2018, 2, 1662-1673.	24.0	297
102	First-principle high-throughput calculations of carrier effective masses of two-dimensional transition metal dichalcogenides. Journal of Semiconductors, 2018, 39, 072001.	3.7	18
103	Rational design of new phases of tin monosulfide by first-principles structure searches. Science China: Physics, Mechanics and Astronomy, 2018, 61, 1.	5.1	15
104	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. Journal of the American Chemical Society, 2017, 139, 2630-2638.	13.7	714
105	Materials discovery at high pressures. Nature Reviews Materials, 2017, 2, .	48.7	427
106	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	8.0	29
107	Computer-Assisted Inverse Design of Inorganic Electrides. Physical Review X, 2017, 7, .	8.9	70
108	Cuâ€"In Halide Perovskite Solar Absorbers. Journal of the American Chemical Society, 2017, 139, 6718-6725.	13.7	316

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109	Highly Oriented Low-Dimensional Tin Halide Perovskites with Enhanced Stability and Photovoltaic Performance. Journal of the American Chemical Society, 2017, 139, 6693-6699.	13.7	723
110	Effects of manganese doping on the structure evolution of small-sized boron clusters. Journal of Physics Condensed Matter, 2017, 29, 265401.	1.8	23
111	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. Journal of Applied Physics, 2017, 121, .	2.5	9
112	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	1.8	31
113	Functionality-Directed Screening of Pb-Free Hybrid Organicâ€“Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. Chemistry of Materials, 2017, 29, 524-538.	6.7	135
114	Discovery and ramifications of incidental MagnÃ©li phase generation and release from industrial coal-burning. Nature Communications, 2017, 8, 194.	12.8	44
115	Doping Lanthanide into Perovskite Nanocrystals: Highly Improved and Expanded Optical Properties. Nano Letters, 2017, 17, 8005-8011.	9.1	672
116	Sn(II)-Containing Phosphates as Optoelectronic Materials. Chemistry of Materials, 2017, 29, 2459-2465.	6.7	17
117	New stable ternary alkaline-earth metal Pb(II) oxides: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ca</mml:mi><mml:mo>/</mml:mo><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaPbO</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review Materials, 2017, 1, .	2.4	10
118	Stability, electronic structures and thermoelectric properties of binary Znâ€“Sb materials. Journal of Materials Chemistry C, 2016, 4, 11305-11312.	5.5	19
119	Design of ternary alkaline-earth metal Sn(<scp>ii</scp>) oxides with potential good p-type conductivity. Journal of Materials Chemistry C, 2016, 4, 4592-4599.	5.5	29
120	Intrinsic ultralow lattice thermal conductivity of the unfilled skutterudite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FeSb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml: Physical Review B, 2016, 94, .	3.2	22
121	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	7.8	132
122	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃. Chemistry of Materials, 2016, 28, 4349-4357.	6.7	139
123	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 597-602.	4.6	100
124	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. Chemistry of Materials, 2016, 28, 1746-1755.	6.7	68
125	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95.	7.5	42
126	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	3.0	138

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127	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	3.3	71
128	Intrinsic Transparent Conductors without Doping. Physical Review Letters, 2015, 115, 176602.	7.8	36
129	N₂H: a novel polymeric hydronitrogen as a high energy density material. Journal of Materials Chemistry A, 2015, 3, 4188-4194.	10.3	49
130	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. APL Materials, 2015, 3, .	5.1	29
131	Evolution of Electronic Structure as a Function of Layer Thickness in Group-VIB Transition Metal Dichalcogenides: Emergence of Localization Prototypes. Nano Letters, 2015, 15, 949-957.	9.1	72
132	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	1.8	93
133	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	5.6	72
134	Reinterpretation of the Expected Electronic Density of States of Semiconductor Nanowires. Nano Letters, 2015, 15, 88-95.	9.1	9
135	Genetic design of enhanced valley splitting towards a spin qubit in silicon. Nature Communications, 2013, 4, 2396.	12.8	49
136	The Birth of a Type-II Nanostructure: Carrier Localization and Optical Properties of Isoelectronically Doped CdSe:Te Nanocrystals. ACS Nano, 2012, 6, 8325-8334.	14.6	15
137	Genomic Design of Strong Direct-Gap Optical Transition in Si/Ge Core/Multishell Nanowires. Nano Letters, 2012, 12, 984-991.	9.1	54
138	Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. Physical Review B, 2011, 84, .	3.2	24
139	Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. Physical Review B, 2011, 84, .	3.2	15
140	Electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CsFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms its alloy with cobalt: A magnetic compound related to the iron superconductors. Physical Review B, 2010, 81, .	3.2	2
141	Electronic structure and thermoelectric properties:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbBi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms related intergrowth compounds. Physical Review B, 2010, 81, .	3.2	56
142	Electronic structure, localization, and spin-state transition in Cu-substituted<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>FeSe</mml:mtext><mml:mo>:</mml:mo><mml:msub><mml:mrow><mml:mtext>Fe</mml:m Physical Review B, 2010, 81, .	3.2	43
143	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, 4055-4060.	9.1	76
144	Zintl-phase compounds with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnSb</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:m anions: Electronic structure and thermoelectric properties. Physical Review B, 2010, 81, .	3.2	66

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145	Density functional study of the overdoped iron chalcogenide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TlFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ThCr</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 80, .	3.2	36
146	Electronic structure and thermoelectric properties of layered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbSe-WSe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2009, 80, .	3.2	57
147	Electronic structure ofBa(Fe,Ru)2As2andSr(Fe,Ir)2As2alloys. Physical Review B, 2009, 79, .	3.2	42
148	Density functional study of the electronic structure and magnetism of LaFeAsO alloyed with Zn. Physical Review B, 2009, 80, .	3.2	24
149	Electronic correlations in the iron pnictides. Nature Physics, 2009, 5, 647-650.	16.7	317
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