Shengli Zhang

List of Publications by Citations

166 papers	10,855 citations	43 h-index	103 g-index
181 ext. papers	13,119 ext. citations	8.5 avg, IF	6.73 L-index

#	Paper	IF	Citations
166	CsPbX3 Quantum Dots for Lighting and Displays: Room-Temperature Synthesis, Photoluminescence Superiorities, Underlying Origins and White Light-Emitting Diodes. *Advanced Functional Materials*, **2016**, 26, 2435-2445	15.6	1548
165	Atomically thin arsenene and antimonene: semimetal-semiconductor and indirect-direct band-gap transitions. *Angewandte Chemie - International Edition*, **2015**, 54, 3112-5	16.4	994
164	Two-dimensional antimonene single crystals grown by van der Waals epitaxy. *Nature Communications*, **2016**, 7, 13352	17.4	633
163	Recent progress in 2D group-VA semiconductors: from theory to experiment. *Chemical Society Reviews*, **2018**, 47, 982-1021	58.5	549
162	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. *Angewandte Chemie - International Edition*, **2016**, 55, 1666-9	16.4	535
161	Engineering surface states of carbon dots to achieve controllable luminescence for solid-luminescent composites and sensitive Be2+ detection. *Scientific Reports*, **2015**, 4,	4.9	447
160	Atomically Thin Arsenene and Antimonene: Semimetal–Semiconductor and Indirect–Direct Band-Gap Transitions. *Angewandte Chemie*, **2015**, 127, 3155-3158	3.6	323
159	Tackling the Activity and Selectivity Challenges of Electrocatalysts toward the Nitrogen Reduction Reaction via Atomically Dispersed Biatom Catalysts. *Journal of the American Chemical Society*, **2020**, 142, 5709-5721	16.4	265
158	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. *Angewandte Chemie*, **2016**, 128, 1698-1701	3.6	254
157	2D V-V Binary Materials: Status and Challenges. *Advanced Materials*, **2019**, 31, e1902352	24	236
156	Antimonene Oxides: Emerging Tunable Direct Bandgap Semiconductor and Novel Topological Insulator. *Nano Letters*, **2017**, 17, 3434-3440	11.5	217
155	CsPbBr Quantum Dots 2.0: Benzenesulfonic Acid Equivalent Ligand Awakens Complete Purification. *Advanced Materials*, **2019**, 31, e1900767	24	189
154	Nonlinear Saturable Absorption of Liquid-Exfoliated Molybdenum/Tungsten Ditelluride Nanosheets. *Small*, **2016**, 12, 1489-97	11	179
153	WS□saturable absorber for dissipative soliton mode locking at 1.06 and 1.55 □m. *Optics Express*, **2015**, 23, 27509-19	3.3	156
152	A promising two-dimensional solar cell donor: Black arsenic–phosphorus monolayer with 1.54 eV direct bandgap and mobility exceeding 14,000 cm2V□1s□1. *Nano Energy*, **2016**, 28, 433-439	17.1	152
151	2D Fe-containing cobalt phosphide/cobalt oxide lateral heterostructure with enhanced activity for oxygen evolution reaction. *Nano Energy*, **2019**, 56, 109-117	17.1	150
150	Boosting Two-Dimensional MoS/CsPbBr Photodetectors via Enhanced Light Absorbance and Interfacial Carrier Separation. *ACS Applied Materials & Interfaces*, **2018**, 10, 2801-2809	9.5	140

149	Few-Layer Antimonene: Anisotropic Expansion and Reversible Crystalline-Phase Evolution Enable Large-Capacity and Long-Life Na-Ion Batteries. *ACS Nano*, **2018**, 12, 1887-1893	16.7	135
148	Lateral black phosphorene PN junctions formed via chemical doping for high performance near-infrared photodetector. *Nano Energy*, **2016**, 25, 34-41	17.1	126
147	Hydrogenated arsenenes as planar magnet and Dirac material. *Applied Physics Letters*, **2015**, 107, 022102	3.4	122
146	Optimizing Hybridization of 1T and 2H Phases in MoS2 Monolayers to Improve Capacitances of Supercapacitors. *Materials Research Letters*, **2015**, 3, 177-183	7.4	121
145	Simultaneously Achieving High Activity and Selectivity toward Two-Electron O2 Electroreduction: The Power of Single-Atom Catalysts. *ACS Catalysis*, **2019**, 9, 11042-11054	13.1	120
144	Black phosphorene as a hole extraction layer boosting solar water splitting of oxygen evolution catalysts. *Nature Communications*, **2019**, 10, 2001	17.4	120
143	GeSe monolayer semiconductor with tunable direct band gap and small carrier effective mass. *Applied Physics Letters*, **2015**, 107, 122107	3.4	116
142	Ab Initio Study of the Adsorption of Small Molecules on Stanene. *Journal of Physical Chemistry C*, **2016**, 120, 13987-13994	3.8	113
141	Semiconductor-topological insulator transition of two-dimensional SbAs induced by biaxial tensile strain. *Physical Review B*, **2016**, 93,	3.3	111
140	Ultrathin Bismuth Nanosheets for Stable Na-Ion Batteries: Clarification of Structure and Phase Transition by in Situ Observation. *Nano Letters*, **2019**, 19, 1118-1123	11.5	93
139	Electronic structure and optical properties of graphene/stanene heterobilayer. *Physical Chemistry Chemical Physics*, **2016**, 18, 16302-9	3.6	91
138	Near-Infrared Plasmonic 2D Semimetals for Applications in Communication and Biology. *Advanced Functional Materials*, **2016**, 26, 1793-1802	15.6	88
137	Two-dimensional BX (X = P, As, Sb) semiconductors with mobilities approaching graphene. *Nanoscale*, **2016**, 8, 13407-13	7.7	84
136	Van der Waals bilayer antimonene: A promising thermophotovoltaic cell material with 31% energy conversion efficiency. *Nano Energy*, **2017**, 38, 561-568	17.1	78
135	Advances of 2D bismuth in energy sciences. *Chemical Society Reviews*, **2020**, 49, 263-285	58.5	78
134	Tunable electronic properties of GeSe/phosphorene heterostructure from first-principles study. *Applied Physics Letters*, **2016**, 109, 103104	3.4	71
133	Near-Complete Suppression of Oxygen Evolution for Photoelectrochemical HO Oxidative HO Synthesis. *Journal of the American Chemical Society*, **2020**, 142, 8641-8648	16.4	68
132	Two-dimensional GeS with tunable electronic properties via external electric field and strain. *Nanotechnology*, **2016**, 27, 274001	3.4	68

131	Modulating Epitaxial Atomic Structure of Antimonene through Interface Design. *Advanced Materials*, **2019**, 31, e1902606	24	63
130	Two-dimensional SiP: an unexplored direct band-gap semiconductor. *2D Materials*, **2017**, 4, 015030	5.9	59
129	Tinene: a two-dimensional Dirac material with a 72 meV band gap. *Physical Chemistry Chemical Physics*, **2015**, 17, 12634-8	3.6	55
128	A High-Performance Nitro-Explosives Schottky Sensor Boosted by Interface Modulation. *Advanced Functional Materials*, **2015**, 25, 4039-4048	15.6	52
127	Recent progress in 2D group IV-IV monochalcogenides: synthesis, properties and applications. *Nanotechnology*, **2019**, 30, 252001	3.4	52
126	Quantum Dots: CsPbX3 Quantum Dots for Lighting and Displays: Room-Temperature Synthesis, Photoluminescence Superiorities, Underlying Origins and White Light-Emitting Diodes (Adv. Funct. Mater. 15/2016). *Advanced Functional Materials*, **2016**, 26, 2584-2584	15.6	48
125	N- and p-type doping of antimonene. *RSC Advances*, **2016**, 6, 14620-14625	3.7	48
124	First-Principles Study of Field Emission Properties of Graphene-ZnO Nanocomposite. *Journal of Physical Chemistry C*, **2010**, 114, 19284-19288	3.8	47
123	Aligned Heterointerface-Induced 1T-MoS Monolayer with Near-Ideal Gibbs Free for Stable Hydrogen Evolution Reaction. *Small*, **2019**, 15, e1804903	11	43
122	A new 2D high-pressure phase of PdSe2 with high-mobility transport anisotropy for photovoltaic applications. *Journal of Materials Chemistry C*, **2019**, 7, 2096-2105	7.1	43
121	Ultrathin tellurium dioxide: emerging direct bandgap semiconductor with high-mobility transport anisotropy. *Nanoscale*, **2018**, 10, 8397-8403	7.7	43
120	Switching excitonic recombination and carrier trapping in cesium lead halide perovskites by air. *Communications Physics*, **2018**, 1,	5.4	43
119	Designing sub-10-nm Metal-Oxide-Semiconductor Field-Effect Transistors via Ballistic Transport and Disparate Effective Mass: The Case of Two-Dimensional BiN. *Physical Review Applied*, **2020**, 13,	4.3	42
118	A class of Pb-free double perovskite halide semiconductors with intrinsic ferromagnetism, large spin splitting and high Curie temperature. *Materials Horizons*, **2018**, 5, 961-968	14.4	40
117	Structural and electronic properties of atomically thin germanium selenide polymorphs. *Science China Materials*, **2015**, 58, 929-935	7.1	38
116	Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction. *Advanced Functional Materials*, **2021**, 31, 2008056	15.6	38
115	Tailoring natural layered Ꞵphase antimony into few layer antimonene for Li storage with high rate capabilities. *Journal of Materials Chemistry A*, **2019**, 7, 3238-3243	13	37
114	The impact of Mg content on the structural, electrical and optical properties of MgZnO alloys: A first principles study. *Current Applied Physics*, **2015**, 15, 423-428	2.6	37

113	Anisotropic In-Plane Ballistic Transport in Monolayer Black Arsenic-Phosphorus FETs. *Advanced Electronic Materials*, **2020**, 6, 1901281	6.4	36
112	Noncovalent Molecular Doping of Two-Dimensional Materials. *ChemNanoMat*, **2015**, 1, 542-557	3.5	35
111	Modulating the phase transition between metallic and semiconducting single-layer MoS2 and WS2 through size effects. *Physical Chemistry Chemical Physics*, **2015**, 17, 1099-105	3.6	35
110	First-principles study of SO2 sensors based on phosphorene and its isoelectronic counterparts: GeS, GeSe, SnS, SnSe. *Chemical Physics Letters*, **2017**, 686, 83-87	2.5	35
109	MoS2 nanoparticles coupled to SnS2 nanosheets: The structural and electronic modulation for synergetic electrocatalytic hydrogen evolution. *Journal of Catalysis*, **2018**, 366, 8-15	7.3	32
108	Identifying electrocatalytic activity and mechanism of Ce1/3NbO3 perovskite for nitrogen reduction to ammonia at ambient conditions. *Applied Catalysis B: Environmental*, **2021**, 280, 119419	21.8	31
107	The effect of electric field on Ti-decorated graphyne for hydrogen storage. *Computational and Theoretical Chemistry*, **2014**, 1035, 68-75	2	30
106	Theoretical investigation of growth, stability, and electronic properties of beaded ZnO nanoclusters. *Journal of Materials Chemistry*, **2011**, 21, 16905		27
105	Mechanistic Understanding of Two-Dimensional Phosphorus, Arsenic, and Antimony High-Capacity Anodes for Fast-Charging Lithium/Sodium Ion Batteries. *Journal of Physical Chemistry C*, **2018**, 122, 29559-29566	3.8	27
104	Quantum confinement effect of two-dimensional all-inorganic halide perovskites. *Science China Materials*, **2017**, 60, 811-818	7.1	26
103	DFT coupled with NEGF study of a promising two-dimensional channel material: black phosphorene-type GaTeCl. *Nanoscale*, **2018**, 10, 3350-3355	7.7	25
102	"Silent" Amino Acid Residues at Key Subunit Interfaces Regulate the Geometry of Protein Nanocages. *ACS Nano*, **2016**, 10, 10382-10388	16.7	25
101	The structural, electrical and optical properties of Mg-doped ZnO with different interstitial Mg concentration. *Materials Chemistry and Physics*, **2016**, 182, 15-21	4.4	24
100	Tunable electronic structure and enhanced optical properties in quasi-metallic hydrogenated/fluorinated SiC heterobilayer. *Journal of Materials Chemistry C*, **2016**, 4, 7406-7414	7.1	23
99	A Perovskite Light-Emitting Device Driven by Low-Frequency Alternating Current Voltage. *Advanced Optical Materials*, **2018**, 6, 1800206	8.1	23
98	A promising two-dimensional channel material: monolayer antimonide phosphorus. *Science China Materials*, **2016**, 59, 648-656	7.1	22
97	Layer-controlled band alignment, work function and optical properties of few-layer GeSe. *Physica B: Condensed Matter*, **2017**, 519, 90-94	2.8	22
96	Ferroelastic lattice rotation and band-gap engineering in quasi 2D layered-structure PdSe under uniaxial stress. *Nanoscale*, **2019**, 11, 12317-12325	7.7	21

95	Influences of Stone–Wales defects on the structure, stability and electronic properties of antimonene: A first principle study. *Physica B: Condensed Matter*, **2016**, 503, 126-129	2.8	21
94	Conversion of the Native 24-mer Ferritin Nanocage into Its Non-Native 16-mer Analogue by Insertion of Extra Amino Acid Residues. *Angewandte Chemie - International Edition*, **2016**, 55, 16064-16070	16.4	21
93	Two-Dimensional Pnictogen for Field-Effect Transistors. *Research*, **2019**, 2019, 1046329	7.8	21
92	Two-Dimensional BAs/InTe: A Promising Tandem Solar Cell with High Power Conversion Efficiency. *ACS Applied Materials & Interfaces*, **2020**, 12, 6074-6081	9.5	20
91	Two-dimensional transition metal diborides: promising Dirac electrocatalysts with large reaction regions toward efficient N2 fixation. *Journal of Materials Chemistry A*, **2019**, 7, 25887-25893	13	20
90	An Ångström-level d-spacing controlling synthetic route for MoS2 towards stable intercalation of sodium ions. *Journal of Materials Chemistry A*, **2018**, 6, 22513-22518	13	20
89	First-principles calculations of the electronic properties of two-dimensional pentagonal structure XS2 (X=Ni, Pd, Pt). *Vacuum*, **2020**, 174, 109176	3.7	19
88	Considering the spin–orbit coupling effect on the photocatalytic performance of AlN/MX2 nanocomposites. *Journal of Materials Chemistry C*, **2017**, 5, 9412-9420	7.1	19
87	Mechanistic investigations on the adsorption of thiophene over Zn3NiO4 bimetallic oxide cluster. *Applied Surface Science*, **2012**, 258, 10148-10153	6.7	19
86	Dipole controlled Schottky barrier in the blue-phosphorene-phase of GeSe based van der Waals heterostructures. *Nanoscale Horizons*, **2019**, 4, 480-489	10.8	19
85	Metallic oxide nanocrystals with near-infrared plasmon resonance for efficient, stable and biocompatible photothermal cancer therapy. *Journal of Materials Chemistry B*, **2017**, 5, 7393-7402	7.3	17
84	Theoretical investigation of adsorption and dissociation of H2 on (ZrO2)n (n=1–8) clusters. *International Journal of Hydrogen Energy*, **2011**, 36, 9069-9078	6.7	17
83	Uncovering the Anisotropic Electronic Structure of 2D Group VA-VA Monolayers for Quantum Transport. *IEEE Electron Device Letters*, **2021**, 42, 66-69	4.4	17
82	Tuning the electronic and optical properties of graphane/silicane and fhBN/silicane nanosheets via interfacial dihydrogen bonding and electrical field control. *Journal of Materials Chemistry C*, **2016**, 4, 8962-8972	7.1	15
81	Unusual Electronic Transitions in Two-dimensional Layered SnSb2Te4 Driven by Electronic State Rehybridization. *Physical Review Applied*, **2019**, 11,	4.3	14
80	Density functional theory studies of Yb-, Ca- and Sr-substituted Mg2NiH4 hydrides. *Computational Materials Science*, **2013**, 74, 55-64	3.2	14
79	Effects of nonmetal element (B, C and Si) additives in Mg2Ni hydrogen storage alloy: A first-principles study. *International Journal of Hydrogen Energy*, **2012**, 37, 6700-6713	6.7	14
78	Field-Emission Mechanism of Island-Shaped Graphene–BN Nanocomposite. *Journal of Physical Chemistry C*, **2011**, 115, 9471-9476	3.8	14

77	Robust two-dimensional topological insulators in derivatives of group-VA oxides with large band gap: Tunable quantum spin Hall states. *Applied Materials Today*, **2019**, 15, 163-170	6.6	13
76	First-principles investigation of thiophene adsorption on Ni13 and Zn@Ni12 nanoclusters. *Computational and Theoretical Chemistry*, **2013**, 1020, 136-142	2	13
75	Beneficial restacking of 2D nanomaterials for electrocatalysis: a case of MoS membranes. *Chemical Communications*, **2020**, 56, 7005-7008	5.8	12
74	Band offsets in new BN/BX (X = P, As, Sb) lateral heterostructures based on bond-orbital theory. *Nanoscale*, **2018**, 10, 15918-15925	7.7	12
73	Significant effects of graphite fragments on hydrogen storage performances of LiBH4: A first-principles approach. *International Journal of Hydrogen Energy*, **2013**, 38, 13717-13727	6.7	12
72	Theoretical investigations of sp-sp2 hybridized zero-dimensional fullerenynes. *Nanoscale*, **2012**, 4, 2839-42	7.7	12
71	First-principles study of structural, electronic and vibrational properties of aluminum-doped silica nanotubes. *Chemical Physics Letters*, **2010**, 498, 172-177	2.5	12
70	Multilayer Cascade Charge Transport Layer for High-Performance Inverted Mesoscopic All-Inorganic and Hybrid Wide-Bandgap Perovskite Solar Cells. *Solar Rrl*, **2020**, 4, 2000344	7.1	12
69	A highly sensitive and selective SnS2 monolayer sensor in detecting SF6 decomposition gas. *Applied Surface Science*, **2021**, 541, 148494	6.7	12
68	Structural, magnetic and electronic properties of FenPt13−n clusters with n=0−13: A first-principle study. *Journal of Magnetism and Magnetic Materials*, **2014**, 369, 27-33	2.8	11
67	First-principles study of cubane-type ZnO: Another ZnO polymorph. *Chemical Physics Letters*, **2013**, 557, 102-105	2.5	11
66	Band engineering realized by chemical combination in 2D group VA−VA materials. *Nanoscale Horizons*, **2019**, 4, 1145-1152	10.8	10
65	The effect of electric field on hydrogen storage for B/N-codoped graphyne. *RSC Advances*, **2014**, 4, 54879-54884	3.7	10
64	Confinement effects on structural, electronic properties and dehydrogenation thermodynamics of LiBH4. *International Journal of Hydrogen Energy*, **2013**, 38, 8367-8375	6.7	10
63	High-performance vertical field-effect transistors based on all-inorganic perovskite microplatelets. *Journal of Materials Chemistry C*, **2020**, 8, 12632-12637	7.1	10
62	Ballistic Transport in High-Performance and Low-Power Sub-5 nm Two-Dimensional ZrNBr MOSFETs. *IEEE Electron Device Letters*, **2020**, 41, 1029-1032	4.4	9
61	Porous silaphosphorene, silaarsenene and silaantimonene: a sweet marriage of Si and P/As/Sb. *Journal of Materials Chemistry A*, **2018**, 6, 3738-3746	13	9
60	Efficient Full-Color Boron Nitride Quantum Dots for Thermostable Flexible Displays. *ACS Nano*, **2021**, 15, 14610-14617	16.7	9

59	Structural transition, metallization, and superconductivity in quasi-two-dimensional layered PdS2 under compression. *Physical Review B*, **2020**, 101,	3.3	8
58	A first-principle study on hydrogen storage of metal atoms (M□=□Li, Ca, Sc, and Ti) coated B40 fullerene composites. *Computational and Theoretical Chemistry*, **2020**, 1181, 112823	2	8
57	Stability enhancement and electronic tunability of two-dimensional SbIV compounds via surface functionalization. *Applied Surface Science*, **2018**, 427, 363-368	6.7	8
56	Modulating tunneling width and energy window for high-on-current two-dimensional tunnel field-effect transistors. *Nano Energy*, **2021**, 81, 105642	17.1	8
55	Ballistic Quantum Transport of Sub-10 nm 2D Sb2Te2Se Transistors. *Advanced Electronic Materials*, **2019**, 5, 1900813	6.4	7
54	Ultrascaled Double-Gate Monolayer SnS2 MOSFETs for High-Performance and Low-Power Applications. *Physical Review Applied*, **2020**, 14,	4.3	7
53	High-performance monolayer NaSb shrinking transistors: a DFT-NEGF study. *Nanoscale*, **2020**, 12, 18931-18937	7.7	7
52	Highly sensitive detection and imaging of ultraviolet-B light for precisely controlling vitamin D generation in the human body. *Journal of Materials Chemistry C*, **2019**, 7, 4503-4508	7.1	6
51	Transferable High-Quality Inorganic Perovskites for Optoelectronic Devices by Weak Interaction Heteroepitaxy. *ACS Applied Materials & Interfaces*, **2020**, 12, 19674-19681	9.5	6
50	Structure, electronic characteristic and thermodynamic properties of K2ZnH4 hydride crystal: A first-principles study. *Journal of Alloys and Compounds*, **2013**, 549, 30-37	5.7	6
49	Theoretical investigation of assembled (CdTe)12N (N = 1□5) multi-cage nanochains. *Computational Materials Science*, **2013**, 68, 238-244	3.2	6
48	New ultra-incompressible phases of NbB4 predicted from first principles. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 362-367	2.3	6
47	Extending Channel Scaling Limit of p-MOSFETs Through Antimonene With Heavy Effective Mass and High Density of State. *IEEE Transactions on Electron Devices*, **2022**, 1-6	2.9	6
46	Ru55 nanoparticles catalyze the dissociation of H2O monomer□and□dimer to produce hydrogen: A comparative DFT□study. *International Journal of Hydrogen Energy*, **2016**, 41, 3844-3853	6.7	5
45	Stabilizing Layered Structure in Aqueous Electrolyte via Dynamic Water Intercalation/Deintercalation.. *Advanced Materials*, **2022**, e2108541	24	5
44	A two-photon tandem black phosphorus quantum dot-sensitized BiVO4 photoanode for solar water splitting. *Energy and Environmental Science*,	35.4	5
43	Topologically protected states and half-metal behaviors: Defect-strain synergy effects in two-dimensional antimonene. *Physical Review Materials*, **2019**, 3,	3.2	5
42	Pentagonal two-dimensional noble-metal dichalcogenide PdSSe for photocatalytic water splitting with pronounced optical absorption and ultrahigh anisotropic carrier mobility. *Journal of Materials Chemistry C*,	7.1	5

41	Defect Regulating of Few-Layer Antimonene from Acid-Assisted Exfoliation for Enhanced Electrocatalytic Nitrogen Fixation. *ACS Applied Materials & Interfaces*, **2021**, 13, 40618-40628	9.5	5
40	Dual In-situ Laser Techniques Underpin the Role of Cations in Impacting Electrocatalysts.. *Angewandte Chemie - International Edition*, **2022**,	16.4	5
39	DFT coupled with NEGF study of the electronic properties and ballistic transport performances of 2D SbSiTe. *Nanoscale*, **2020**, 12, 9958-9963	7.7	4
38	Cu2O□Cu2Se Mixed-Phase Nanoflake Arrays: pH-Universal Hydrogen Evolution Reactions with Ultralow Overpotential. *ChemElectroChem*, **2019**, 6, 5014-5021	4.3	4
37	Dipole-Engineering Strategy for Regulating the Electronic Contact of a Two-Dimensional Sb X /Graphene (X = P , . *Physical Review Applied*, **2022**, 17,	4.3	4
36	Charge-carrier dynamics and regulation strategies in perovskite light-emitting diodes: From materials to devices. *Applied Physics Reviews*, **2022**, 9, 021308	17.3	4
35	Revealing the weak Fermi level pinning effect of 2D semiconductor/2D metal contact: A case of monolayer In2Ge2Te6 and its Janus structure In2Ge2Te3Se3. *Materials Today Physics*, **2022**, 100749	8	4
34	Electronic band structures and optical properties of atomically thin AuSe: first-principle calculations. *Journal of Semiconductors*, **2019**, 40, 062004	2.3	3
33	Theoretical insights into the CO dimerization and trimerization on Pt nanocluster. *RSC Advances*, **2016**, 6, 4354-4364	3.7	3
32	Structural, electronic and thermodynamic properties of R3ZnH5 (R=K, Rb, Cs): A first-principle calculation. *Journal of Solid State Chemistry*, **2013**, 198, 433-439	3.3	3
31	Pressurized Alloying Assisted Synthesis of High Quality Antimonene for Capacitive Deionization. *Advanced Functional Materials*, **2021**, 31, 2102766	15.6	3
30	Conversion of the Native 24-mer Ferritin Nanocage into Its Non-Native 16-mer Analogue by Insertion of Extra Amino Acid Residues. *Angewandte Chemie*, **2016**, 128, 16298-16304	3.6	3
29	Pressure-dependent structural, electronic and optical properties of ZnO with native defect: A first-principles study. *Modern Physics Letters B*, **2016**, 30, 1650275	1.6	3
28	Donor□cceptor units modulate the electronic and photoluminescence characteristics of thiophene oligomers. *Journal of Applied Physics*, **2019**, 126, 245501	2.5	3
27	Halide ion migration in lead-free all-inorganic cesium tin perovskites. *Applied Physics Letters*, **2021**, 119, 031902	3.4	3
26	The electronic properties tuned by the phase transition between the semiconducting and metallic phase of monolayer MoS2/WS2. *Phase Transitions*, **2015**, 88, 726-734	1.3	2
25	Molecular Dynamics Simulations of Silica Nanotube: Structural and Vibrational Properties Under Different Temperatures. *Chinese Journal of Chemical Physics*, **2010**, 23, 497-503	0.9	2
24	Sensing Performance of SO□SO□and NO□Gas Molecules on 2D Pentagonal PdSe□A First-Principle Study. *IEEE Electron Device Letters*, **2021**, 42, 573-576	4.4	2

23	In-Situ and Reversible Enhancement of Photoluminescence from CsPbBr3 Nanoplatelets by Electrical Bias. *Advanced Optical Materials*, **2021**, 9, 2100346	8.1	2
22	Electronic structure and transport properties of 2D RhTeCl: a NEGF-DFT study. *Nanoscale*, **2019**, 11, 20461-20466	7.7	2
21	Tunable conductance and spin filtering in twisted bilayer copper phthalocyanine molecular devices. *Nanoscale Advances*, **2021**, 3, 3497-3501	5.1	2
20	Facet-induced coordination competition for highly ordered CsPbBr3 nanoplatelets with strong polarized emission. *Nano Research*,1	10	2
19	Boosting Alkaline Hydrogen Evolution on Stoichiometric Molybdenum Carbonitride via an Interstitial Vacancy-Elimination Strategy. *Advanced Energy Materials*,2200974	21.8	2
18	Fluorosilicene/chlorosilicene bilayer semiconductor with tunable electronic and optical properties. *Journal of Applied Physics*, **2017**, 121, 055701	2.5	1
17	Physical properties of tetragonal transition-metal borides Nb 2 MB 2 (M□=□Mo, W, Re or Os) with a new superstructure. *Current Applied Physics*, **2015**, 15, 970-976	2.6	1
16	First-principles study on the electronic structures and contact properties of graphene/XC (X = P, As, Sb, and Bi) van der Waals heterostructures. *Physical Chemistry Chemical Physics*, **2021**, 23, 25136-25142	3.6	1
15	First-principle study of puckered arsenene MOSFET. *Journal of Semiconductors*, **2020**, 41, 082006	2.3	1
14	Quantum Transport in Monolayer □CS Field-Effect Transistors. *Advanced Electronic Materials*, **2021**, 7, 2001169	6.4	1
13	Research on metallic chalcogen-functionalized monolayer-puckered V2CX2 (X = S, Se, and Te) as promising Li-ion battery anode materials. *Materials Chemistry Frontiers*, **2021**, 5, 4672-4681	7.8	1
12	Optical detection of quantum geometric tensor in intrinsic semiconductors. *Science China: Physics, Mechanics and Astronomy*, **2021**, 64, 1	3.6	1
11	Tunable giant magnetoresistance ratio in bilayer CuPc molecular devices.. *RSC Advances*, **2022**, 12, 3386-3393	3.7	0
10	A mixed-dimensional WS2/GaSb heterojunction for high-performance p□ diodes and junction field-effect transistors. *Journal of Materials Chemistry C*, **2022**, 10, 1511-1516	7.1	0
9	Unexpected band gap evolution and high carrier mobility sparked by the orbital variation in two-dimensional GaGeX (X = S, Se, Te). *Physica E: Low-Dimensional Systems and Nanostructures*, **2022**, 138, 115112	3	0
8	DFT coupled with NEGF study of structural, electronic and transport properties of two-dimensional InOBr. *Vacuum*, **2020**, 182, 109745	3.7	0
7	Influences of the Pb 6s2 lone pair effect and quantum size effect on the diffusion of oxygen atoms on Pb(111) films. *RSC Advances*, **2016**, 6, 78755-78761	3.7	0
6	Electronic Structure and Quantum Transport Properties of 2D SiP: A First-Principles Study. *Journal of Electronic Materials*, **2021**, 50, 5499-5506	1.9	0

5	A Machine Learning Approach for Optimization of Channel Geometry and Source/Drain Doping Profile of Stacked Nanosheet Transistors. *IEEE Transactions on Electron Devices*, **2022**, 1-7	2.9	0
4	Nanosensors: A High-Performance Nitro-Explosives Schottky Sensor Boosted by Interface Modulation (Adv. Funct. Mater. 26/2015). *Advanced Functional Materials*, **2015**, 25, 4038-4038	15.6	
3	Optical-field induced SU(2) pair potential in caesium lead halide perovskites. *International Journal of Modern Physics B*, **2021**, 35, 2150030	1.1	
2	Structural and electronic properties of KY(BH): DFT+U study.. *RSC Advances*, **2018**, 8, 34374-34379	3.7	
1	Bismuthene **2022**, 173-196		