

Shengli Zhang

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/9565936/shengli-zhang-publications-by-year.pdf>

Version: 2024-04-27

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Stabilizing Layered Structure in Aqueous Electrolyte via Dynamic Water Intercalation/Deintercalation.. <i>Advanced Materials</i> , 2022 , e2108541	24	5
165	Tunable giant magnetoresistance ratio in bilayer CuPc molecular devices.. <i>RSC Advances</i> , 2022 , 12, 3386-3393	3.7	0
164	A mixed-dimensional WS ₂ /GaSb heterojunction for high-performance p _n diodes and junction field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2022 , 10, 1511-1516	7.1	0
163	Extending Channel Scaling Limit of p-MOSFETs Through Antimonene With Heavy Effective Mass and High Density of State. <i>IEEE Transactions on Electron Devices</i> , 2022 , 1-6	2.9	6
162	Unexpected band gap evolution and high carrier mobility sparked by the orbital variation in two-dimensional GaGeX (X = S, Se, Te). <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022 , 138, 115112	3	0
161	Dual In-situ Laser Techniques Underpin the Role of Cations in Impacting Electrocatalysts.. <i>Angewandte Chemie - International Edition</i> , 2022 ,	16.4	5
160	Dipole-Engineering Strategy for Regulating the Electronic Contact of a Two-Dimensional Sb X /Graphene (X = P, As, Sb, Bi). <i>Physical Review Applied</i> , 2022 , 17,	4.3	4
159	Charge-carrier dynamics and regulation strategies in perovskite light-emitting diodes: From materials to devices. <i>Applied Physics Reviews</i> , 2022 , 9, 021308	17.3	4
158	A Machine Learning Approach for Optimization of Channel Geometry and Source/Drain Doping Profile of Stacked Nanosheet Transistors. <i>IEEE Transactions on Electron Devices</i> , 2022 , 1-7	2.9	0
157	Revealing the weak Fermi level pinning effect of 2D semiconductor/2D metal contact: A case of monolayer In ₂ Ge ₂ Te ₆ and its Janus structure In ₂ Ge ₂ Te ₃ Se ₃ . <i>Materials Today Physics</i> , 2022 , 100749	8	4
156	Bismuthene 2022 , 173-196		
155	First-principles study on the electronic structures and contact properties of graphene/XC (X = P, As, Sb, and Bi) van der Waals heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 25136-25142	3.6	1
154	Optical-field induced SU(2) pair potential in caesium lead halide perovskites. <i>International Journal of Modern Physics B</i> , 2021 , 35, 2150030	1.1	
153	Quantum Transport in Monolayer HCS Field-Effect Transistors. <i>Advanced Electronic Materials</i> , 2021 , 7, 2001169	6.4	1
152	Sensing Performance of SO ₂ and NO ₂ Gas Molecules on 2D Pentagonal PdSe ₂ : A First-Principle Study. <i>IEEE Electron Device Letters</i> , 2021 , 42, 573-576	4.4	2
151	In-Situ and Reversible Enhancement of Photoluminescence from CsPbBr ₃ Nanoplatelets by Electrical Bias. <i>Advanced Optical Materials</i> , 2021 , 9, 2100346	8.1	2
150	Pressurized Alloying Assisted Synthesis of High Quality Antimonene for Capacitive Deionization. <i>Advanced Functional Materials</i> , 2021 , 31, 2102766	15.6	3

149	Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction. <i>Advanced Functional Materials</i> , 2021 , 31, 2008056	15.6	38
148	Identifying electrocatalytic activity and mechanism of Ce ₁ /3NbO ₃ perovskite for nitrogen reduction to ammonia at ambient conditions. <i>Applied Catalysis B: Environmental</i> , 2021 , 280, 119419	21.8	31
147	Modulating tunneling width and energy window for high-on-current two-dimensional tunnel field-effect transistors. <i>Nano Energy</i> , 2021 , 81, 105642	17.1	8
146	A highly sensitive and selective SnS ₂ monolayer sensor in detecting SF ₆ decomposition gas. <i>Applied Surface Science</i> , 2021 , 541, 148494	6.7	12
145	Uncovering the Anisotropic Electronic Structure of 2D Group VA-VA Monolayers for Quantum Transport. <i>IEEE Electron Device Letters</i> , 2021 , 42, 66-69	4.4	17
144	Research on metallic chalcogen-functionalized monolayer-puckered V ₂ CX ₂ (X = S, Se, and Te) as promising Li-ion battery anode materials. <i>Materials Chemistry Frontiers</i> , 2021 , 5, 4672-4681	7.8	1
143	Tunable conductance and spin filtering in twisted bilayer copper phthalocyanine molecular devices. <i>Nanoscale Advances</i> , 2021 , 3, 3497-3501	5.1	2
142	Electronic Structure and Quantum Transport Properties of 2D SiP: A First-Principles Study. <i>Journal of Electronic Materials</i> , 2021 , 50, 5499-5506	1.9	0
141	Efficient Full-Color Boron Nitride Quantum Dots for Thermostable Flexible Displays. <i>ACS Nano</i> , 2021 , 15, 14610-14617	16.7	9
140	Halide ion migration in lead-free all-inorganic cesium tin perovskites. <i>Applied Physics Letters</i> , 2021 , 119, 031902	3.4	3
139	Defect Regulating of Few-Layer Antimonene from Acid-Assisted Exfoliation for Enhanced Electrocatalytic Nitrogen Fixation. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 40618-40628	9.5	5
138	Optical detection of quantum geometric tensor in intrinsic semiconductors. <i>Science China: Physics, Mechanics and Astronomy</i> , 2021 , 64, 1	3.6	1
137	Beneficial restacking of 2D nanomaterials for electrocatalysis: a case of MoS membranes. <i>Chemical Communications</i> , 2020 , 56, 7005-7008	5.8	12
136	Structural transition, metallization, and superconductivity in quasi-two-dimensional layered PdS ₂ under compression. <i>Physical Review B</i> , 2020 , 101,	3.3	8
135	Ballistic Transport in High-Performance and Low-Power Sub-5 nm Two-Dimensional ZrNBr MOSFETs. <i>IEEE Electron Device Letters</i> , 2020 , 41, 1029-1032	4.4	9
134	Near-Complete Suppression of Oxygen Evolution for Photoelectrochemical H ₂ O Oxidative H ₂ O ₂ Synthesis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8641-8648	16.4	68
133	Tackling the Activity and Selectivity Challenges of Electrocatalysts toward the Nitrogen Reduction Reaction via Atomically Dispersed Biatom Catalysts. <i>Journal of the American Chemical Society</i> , 2020 , 142, 5709-5721	16.4	265
132	First-principles calculations of the electronic properties of two-dimensional pentagonal structure XS ₂ (X=Ni, Pd, Pt). <i>Vacuum</i> , 2020 , 174, 109176	3.7	19

131	Anisotropic In-Plane Ballistic Transport in Monolayer Black Arsenic-Phosphorus FETs. <i>Advanced Electronic Materials</i> , 2020 , 6, 1901281	6.4	36
130	Two-Dimensional BAs/InTe: A Promising Tandem Solar Cell with High Power Conversion Efficiency. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 6074-6081	9.5	20
129	Designing sub-10-nm Metal-Oxide-Semiconductor Field-Effect Transistors via Ballistic Transport and Disparate Effective Mass: The Case of Two-Dimensional BiN. <i>Physical Review Applied</i> , 2020 , 13,	4.3	42
128	Transferable High-Quality Inorganic Perovskites for Optoelectronic Devices by Weak Interaction Heteroepitaxy. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 19674-19681	9.5	6
127	DFT coupled with NEGF study of the electronic properties and ballistic transport performances of 2D SbSiTe. <i>Nanoscale</i> , 2020 , 12, 9958-9963	7.7	4
126	A first-principle study on hydrogen storage of metal atoms (M=Li, Ca, Sc, and Ti) coated B40 fullerene composites. <i>Computational and Theoretical Chemistry</i> , 2020 , 1181, 112823	2	8
125	Advances of 2D bismuth in energy sciences. <i>Chemical Society Reviews</i> , 2020 , 49, 263-285	58.5	78
124	DFT coupled with NEGF study of structural, electronic and transport properties of two-dimensional InOBr. <i>Vacuum</i> , 2020 , 182, 109745	3.7	0
123	High-performance vertical field-effect transistors based on all-inorganic perovskite microplatelets. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 12632-12637	7.1	10
122	Multilayer Cascade Charge Transport Layer for High-Performance Inverted Mesoscopic All-Inorganic and Hybrid Wide-Bandgap Perovskite Solar Cells. <i>Solar Rrl</i> , 2020 , 4, 2000344	7.1	12
121	First-principle study of puckered arsenene MOSFET. <i>Journal of Semiconductors</i> , 2020 , 41, 082006	2.3	1
120	Ultrascaled Double-Gate Monolayer SnS ₂ MOSFETs for High-Performance and Low-Power Applications. <i>Physical Review Applied</i> , 2020 , 14,	4.3	7
119	High-performance monolayer NaSb shrinking transistors: a DFT-NEGF study. <i>Nanoscale</i> , 2020 , 12, 18931-18937	7.7	7
118	Simultaneously Achieving High Activity and Selectivity toward Two-Electron O ₂ Electroreduction: The Power of Single-Atom Catalysts. <i>ACS Catalysis</i> , 2019 , 9, 11042-11054	13.1	120
117	Tailoring natural layered ϵ -phase antimony into few layer antimonene for Li storage with high rate capabilities. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 3238-3243	13	37
116	Aligned Heterointerface-Induced 1T-MoS Monolayer with Near-Ideal Gibbs Free for Stable Hydrogen Evolution Reaction. <i>Small</i> , 2019 , 15, e1804903	11	43
115	Ultrathin Bismuth Nanosheets for Stable Na-Ion Batteries: Clarification of Structure and Phase Transition by in Situ Observation. <i>Nano Letters</i> , 2019 , 19, 1118-1123	11.5	93
114	Robust two-dimensional topological insulators in derivatives of group-VA oxides with large band gap: Tunable quantum spin Hall states. <i>Applied Materials Today</i> , 2019 , 15, 163-170	6.6	13

113	A new 2D high-pressure phase of PdSe ₂ with high-mobility transport anisotropy for photovoltaic applications. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 2096-2105	7.1	43
112	Unusual Electronic Transitions in Two-dimensional Layered SnSb ₂ Te ₄ Driven by Electronic State Rehybridization. <i>Physical Review Applied</i> , 2019 , 11,	4.3	14
111	Ferroelastic lattice rotation and band-gap engineering in quasi 2D layered-structure PdSe under uniaxial stress. <i>Nanoscale</i> , 2019 , 11, 12317-12325	7.7	21
110	Electronic band structures and optical properties of atomically thin AuSe: first-principle calculations. <i>Journal of Semiconductors</i> , 2019 , 40, 062004	2.3	3
109	Modulating Epitaxial Atomic Structure of Antimonene through Interface Design. <i>Advanced Materials</i> , 2019 , 31, e1902606	24	63
108	CsPbBr Quantum Dots 2.0: Benzenesulfonic Acid Equivalent Ligand Awakens Complete Purification. <i>Advanced Materials</i> , 2019 , 31, e1900767	24	189
107	Band engineering realized by chemical combination in 2D group VAV ₃ materials. <i>Nanoscale Horizons</i> , 2019 , 4, 1145-1152	10.8	10
106	Black phosphorene as a hole extraction layer boosting solar water splitting of oxygen evolution catalysts. <i>Nature Communications</i> , 2019 , 10, 2001	17.4	120
105	Highly sensitive detection and imaging of ultraviolet-B light for precisely controlling vitamin D generation in the human body. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 4503-4508	7.1	6
104	2D V-V Binary Materials: Status and Challenges. <i>Advanced Materials</i> , 2019 , 31, e1902352	24	236
103	Cu ₂ O/Tu ₂ Se Mixed-Phase Nanoflake Arrays: pH-Universal Hydrogen Evolution Reactions with Ultralow Overpotential. <i>ChemElectroChem</i> , 2019 , 6, 5014-5021	4.3	4
102	Ballistic Quantum Transport of Sub-10 nm 2D Sb ₂ Te ₂ Se Transistors. <i>Advanced Electronic Materials</i> , 2019 , 5, 1900813	6.4	7
101	Topologically protected states and half-metal behaviors: Defect-strain synergy effects in two-dimensional antimonene. <i>Physical Review Materials</i> , 2019 , 3,	3.2	5
100	Two-Dimensional Pnictogen for Field-Effect Transistors. <i>Research</i> , 2019 , 2019, 1046329	7.8	21
99	Recent progress in 2D group IV-IV monochalcogenides: synthesis, properties and applications. <i>Nanotechnology</i> , 2019 , 30, 252001	3.4	52
98	Donor-Acceptor units modulate the electronic and photoluminescence characteristics of thiophene oligomers. <i>Journal of Applied Physics</i> , 2019 , 126, 245501	2.5	3
97	Electronic structure and transport properties of 2D RhTeCl: a NEGF-DFT study. <i>Nanoscale</i> , 2019 , 11, 204617-20466	6.7	20466
96	Two-dimensional transition metal diborides: promising Dirac electrocatalysts with large reaction regions toward efficient N ₂ fixation. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 25887-25893	13	20

95	2D Fe-containing cobalt phosphide/cobalt oxide lateral heterostructure with enhanced activity for oxygen evolution reaction. <i>Nano Energy</i> , 2019 , 56, 109-117	17.1	150
94	Dipole controlled Schottky barrier in the blue-phosphorene-phase of GeSe based van der Waals heterostructures. <i>Nanoscale Horizons</i> , 2019 , 4, 480-489	10.8	19
93	Ultrathin tellurium dioxide: emerging direct bandgap semiconductor with high-mobility transport anisotropy. <i>Nanoscale</i> , 2018 , 10, 8397-8403	7.7	43
92	Few-Layer Antimonene: Anisotropic Expansion and Reversible Crystalline-Phase Evolution Enable Large-Capacity and Long-Life Na-Ion Batteries. <i>ACS Nano</i> , 2018 , 12, 1887-1893	16.7	135
91	Porous silaphosphorene, silaarsenene and silaantimonene: a sweet marriage of Si and P/As/Sb. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 3738-3746	13	9
90	DFT coupled with NEGF study of a promising two-dimensional channel material: black phosphorene-type GaTeCl. <i>Nanoscale</i> , 2018 , 10, 3350-3355	7.7	25
89	Boosting Two-Dimensional MoS/CsPbBr Photodetectors via Enhanced Light Absorbance and Interfacial Carrier Separation. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 2801-2809	9.5	140
88	Recent progress in 2D group-VA semiconductors: from theory to experiment. <i>Chemical Society Reviews</i> , 2018 , 47, 982-1021	58.5	549
87	Stability enhancement and electronic tunability of two-dimensional SbIV compounds via surface functionalization. <i>Applied Surface Science</i> , 2018 , 427, 363-368	6.7	8
86	A class of Pb-free double perovskite halide semiconductors with intrinsic ferromagnetism, large spin splitting and high Curie temperature. <i>Materials Horizons</i> , 2018 , 5, 961-968	14.4	40
85	Band offsets in new BN/BX (X = P, As, Sb) lateral heterostructures based on bond-orbital theory. <i>Nanoscale</i> , 2018 , 10, 15918-15925	7.7	12
84	MoS2 nanoparticles coupled to SnS2 nanosheets: The structural and electronic modulation for synergetic electrocatalytic hydrogen evolution. <i>Journal of Catalysis</i> , 2018 , 366, 8-15	7.3	32
83	Structural and electronic properties of KY(BH): DFT+U study.. <i>RSC Advances</i> , 2018 , 8, 34374-34379	3.7	
82	An Ågström-level d-spacing controlling synthetic route for MoS2 towards stable intercalation of sodium ions. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 22513-22518	13	20
81	Mechanistic Understanding of Two-Dimensional Phosphorus, Arsenic, and Antimony High-Capacity Anodes for Fast-Charging Lithium/Sodium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 29559-29567	3.8	27
80	Switching excitonic recombination and carrier trapping in cesium lead halide perovskites by air. <i>Communications Physics</i> , 2018 , 1,	5.4	43
79	A Perovskite Light-Emitting Device Driven by Low-Frequency Alternating Current Voltage. <i>Advanced Optical Materials</i> , 2018 , 6, 1800206	8.1	23
78	Fluorosilicene/chlorosilicene bilayer semiconductor with tunable electronic and optical properties. <i>Journal of Applied Physics</i> , 2017 , 121, 055701	2.5	1

77	Antimonene Oxides: Emerging Tunable Direct Bandgap Semiconductor and Novel Topological Insulator. <i>Nano Letters</i> , 2017 , 17, 3434-3440	11.5	217
76	Van der Waals bilayer antimonene: A promising thermophotovoltaic cell material with 31% energy conversion efficiency. <i>Nano Energy</i> , 2017 , 38, 561-568	17.1	78
75	Two-dimensional SiP: an unexplored direct band-gap semiconductor. <i>2D Materials</i> , 2017 , 4, 015030	5.9	59
74	First-principles study of SO ₂ sensors based on phosphorene and its isoelectronic counterparts: GeS, GeSe, SnS, SnSe. <i>Chemical Physics Letters</i> , 2017 , 686, 83-87	2.5	35
73	Considering the spin-orbit coupling effect on the photocatalytic performance of AlN/MX ₂ nanocomposites. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 9412-9420	7.1	19
72	Quantum confinement effect of two-dimensional all-inorganic halide perovskites. <i>Science China Materials</i> , 2017 , 60, 811-818	7.1	26
71	Metallic oxide nanocrystals with near-infrared plasmon resonance for efficient, stable and biocompatible photothermal cancer therapy. <i>Journal of Materials Chemistry B</i> , 2017 , 5, 7393-7402	7.3	17
70	Layer-controlled band alignment, work function and optical properties of few-layer GeSe. <i>Physica B: Condensed Matter</i> , 2017 , 519, 90-94	2.8	22
69	New ultra-incompressible phases of NbB ₄ predicted from first principles. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017 , 381, 362-367	2.3	6
68	A promising two-dimensional channel material: monolayer antimonide phosphorus. <i>Science China Materials</i> , 2016 , 59, 648-656	7.1	22
67	Influences of Stone-Wales defects on the structure, stability and electronic properties of antimonene: A first principle study. <i>Physica B: Condensed Matter</i> , 2016 , 503, 126-129	2.8	21
66	The structural, electrical and optical properties of Mg-doped ZnO with different interstitial Mg concentration. <i>Materials Chemistry and Physics</i> , 2016 , 182, 15-21	4.4	24
65	Conversion of the Native 24-mer Ferritin Nanocage into Its Non-Native 16-mer Analogue by Insertion of Extra Amino Acid Residues. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 16064-16070	16.4	21
64	Semiconductor-topological insulator transition of two-dimensional SbAs induced by biaxial tensile strain. <i>Physical Review B</i> , 2016 , 93,	3.3	111
63	Two-dimensional antimonene single crystals grown by van der Waals epitaxy. <i>Nature Communications</i> , 2016 , 7, 13352	17.4	633
62	"Silent" Amino Acid Residues at Key Subunit Interfaces Regulate the Geometry of Protein Nanocages. <i>ACS Nano</i> , 2016 , 10, 10382-10388	16.7	25
61	Nonlinear Saturable Absorption of Liquid-Exfoliated Molybdenum/Tungsten DiteLLuride Nanosheets. <i>Small</i> , 2016 , 12, 1489-97	11	179
60	Ab Initio Study of the Adsorption of Small Molecules on Stanene. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 13987-13994	3.8	113

59	Two-dimensional BX (X = P, As, Sb) semiconductors with mobilities approaching graphene. <i>Nanoscale</i> , 2016 , 8, 13407-13	7.7	84
58	Near-Infrared Plasmonic 2D Semimetals for Applications in Communication and Biology. <i>Advanced Functional Materials</i> , 2016 , 26, 1793-1802	15.6	88
57	CsPbX ₃ Quantum Dots for Lighting and Displays: Room-Temperature Synthesis, Photoluminescence Superiorities, Underlying Origins and White Light-Emitting Diodes. <i>Advanced Functional Materials</i> , 2016 , 26, 2435-2445	15.6	1548
56	Quantum Dots: CsPbX ₃ Quantum Dots for Lighting and Displays: Room-Temperature Synthesis, Photoluminescence Superiorities, Underlying Origins and White Light-Emitting Diodes (Adv. Funct. Mater. 15/2016). <i>Advanced Functional Materials</i> , 2016 , 26, 2584-2584	15.6	48
55	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 1666-9	16.4	535
54	N- and p-type doping of antimonene. <i>RSC Advances</i> , 2016 , 6, 14620-14625	3.7	48
53	Ru ₅₅ nanoparticles catalyze the dissociation of H ₂ O monomer and dimer to produce hydrogen: A comparative DFT study. <i>International Journal of Hydrogen Energy</i> , 2016 , 41, 3844-3853	6.7	5
52	Theoretical insights into the CO dimerization and trimerization on Pt nanocluster. <i>RSC Advances</i> , 2016 , 6, 4354-4364	3.7	3
51	Tunable electronic structure and enhanced optical properties in quasi-metallic hydrogenated/fluorinated SiC heterobilayer. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 7406-7414	7.1	23
50	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. <i>Angewandte Chemie</i> , 2016 , 128, 1698-1701	3.6	254
49	Conversion of the Native 24-mer Ferritin Nanocage into Its Non-Native 16-mer Analogue by Insertion of Extra Amino Acid Residues. <i>Angewandte Chemie</i> , 2016 , 128, 16298-16304	3.6	3
48	Tunable electronic properties of GeSe/phosphorene heterostructure from first-principles study. <i>Applied Physics Letters</i> , 2016 , 109, 103104	3.4	71
47	Two-dimensional GeS with tunable electronic properties via external electric field and strain. <i>Nanotechnology</i> , 2016 , 27, 274001	3.4	68
46	Lateral black phosphorene PN junctions formed via chemical doping for high performance near-infrared photodetector. <i>Nano Energy</i> , 2016 , 25, 34-41	17.1	126
45	Electronic structure and optical properties of graphene/stanene heterobilayer. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 16302-9	3.6	91
44	Tuning the electronic and optical properties of graphene/silicane and fhBN/silicane nanosheets via interfacial dihydrogen bonding and electrical field control. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 8962-8972 ¹⁵	7.1	15
43	A promising two-dimensional solar cell donor: Black arsenic-phosphorus monolayer with 1.54 eV direct bandgap and mobility exceeding 14,000 cm ² V ⁻¹ s ⁻¹ . <i>Nano Energy</i> , 2016 , 28, 433-439	17.1	152
42	Pressure-dependent structural, electronic and optical properties of ZnO with native defect: A first-principles study. <i>Modern Physics Letters B</i> , 2016 , 30, 1650275	1.6	3

41	Influences of the Pb 6s ² lone pair effect and quantum size effect on the diffusion of oxygen atoms on Pb(111) films. <i>RSC Advances</i> , 2016 , 6, 78755-78761	3.7	0
40	Optimizing Hybridization of 1T and 2H Phases in MoS ₂ Monolayers to Improve Capacitances of Supercapacitors. <i>Materials Research Letters</i> , 2015 , 3, 177-183	7.4	121
39	Physical properties of tetragonal transition-metal borides Nb ₂ MB ₂ (M=Mo, W, Re or Os) with a new superstructure. <i>Current Applied Physics</i> , 2015 , 15, 970-976	2.6	1
38	The electronic properties tuned by the phase transition between the semiconducting and metallic phase of monolayer MoS ₂ /WS ₂ . <i>Phase Transitions</i> , 2015 , 88, 726-734	1.3	2
37	Tinene: a two-dimensional Dirac material with a 72 meV band gap. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 12634-8	3.6	55
36	Noncovalent Molecular Doping of Two-Dimensional Materials. <i>ChemNanoMat</i> , 2015 , 1, 542-557	3.5	35
35	Hydrogenated arsenenes as planar magnet and Dirac material. <i>Applied Physics Letters</i> , 2015 , 107, 022102	3.4	122
34	Modulating the phase transition between metallic and semiconducting single-layer MoS ₂ and WS ₂ through size effects. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 1099-105	3.6	35
33	Engineering surface states of carbon dots to achieve controllable luminescence for solid-luminescent composites and sensitive Be ²⁺ detection. <i>Scientific Reports</i> , 2015 , 4,	4.9	447
32	Nanosensors: A High-Performance Nitro-Explosives Schottky Sensor Boosted by Interface Modulation (Adv. Funct. Mater. 26/2015). <i>Advanced Functional Materials</i> , 2015 , 25, 4038-4038	15.6	
31	GeSe monolayer semiconductor with tunable direct band gap and small carrier effective mass. <i>Applied Physics Letters</i> , 2015 , 107, 122107	3.4	116
30	WS ₂ saturable absorber for dissipative soliton mode locking at 1.06 and 1.55 μm. <i>Optics Express</i> , 2015 , 23, 27509-19	3.3	156
29	A High-Performance Nitro-Explosives Schottky Sensor Boosted by Interface Modulation. <i>Advanced Functional Materials</i> , 2015 , 25, 4039-4048	15.6	52
28	Structural and electronic properties of atomically thin germanium selenide polymorphs. <i>Science China Materials</i> , 2015 , 58, 929-935	7.1	38
27	The impact of Mg content on the structural, electrical and optical properties of MgZnO alloys: A first principles study. <i>Current Applied Physics</i> , 2015 , 15, 423-428	2.6	37
26	Atomically thin arsenene and antimonene: semimetal-semiconductor and indirect-direct band-gap transitions. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 3112-5	16.4	994
25	Atomically Thin Arsenene and Antimonene: Semimetal-Semiconductor and Indirect-Direct Band-Gap Transitions. <i>Angewandte Chemie</i> , 2015 , 127, 3155-3158	3.6	323
24	The effect of electric field on hydrogen storage for B/N-codoped graphyne. <i>RSC Advances</i> , 2014 , 4, 54879-54884	3.5	40

23	Structural, magnetic and electronic properties of $\text{Fe}_n\text{Pt}_{13-n}$ clusters with $n=0-13$: A first-principle study. <i>Journal of Magnetism and Magnetic Materials</i> , 2014 , 369, 27-33	2.8	11
22	The effect of electric field on Ti-decorated graphyne for hydrogen storage. <i>Computational and Theoretical Chemistry</i> , 2014 , 1035, 68-75	2	30
21	First-principles investigation of thiophene adsorption on Ni_{13} and Zn@Ni_{12} nanoclusters. <i>Computational and Theoretical Chemistry</i> , 2013 , 1020, 136-142	2	13
20	Structural, electronic and thermodynamic properties of R_3ZnH_5 ($\text{R}=\text{K}, \text{Rb}, \text{Cs}$): A first-principle calculation. <i>Journal of Solid State Chemistry</i> , 2013 , 198, 433-439	3.3	3
19	First-principles study of cubane-type ZnO: Another ZnO polymorph. <i>Chemical Physics Letters</i> , 2013 , 557, 102-105	2.5	11
18	Structure, electronic characteristic and thermodynamic properties of K_2ZnH_4 hydride crystal: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2013 , 549, 30-37	5.7	6
17	Theoretical investigation of assembled $(\text{CdTe})_{12N}$ ($N = 1-5$) multi-cage nanochains. <i>Computational Materials Science</i> , 2013 , 68, 238-244	3.2	6
16	Confinement effects on structural, electronic properties and dehydrogenation thermodynamics of LiBH_4 . <i>International Journal of Hydrogen Energy</i> , 2013 , 38, 8367-8375	6.7	10
15	Significant effects of graphite fragments on hydrogen storage performances of LiBH_4 : A first-principles approach. <i>International Journal of Hydrogen Energy</i> , 2013 , 38, 13717-13727	6.7	12
14	Density functional theory studies of Yb-, Ca- and Sr-substituted Mg_2NiH_4 hydrides. <i>Computational Materials Science</i> , 2013 , 74, 55-64	3.2	14
13	Theoretical investigations of sp-sp ² hybridized zero-dimensional fullerenynes. <i>Nanoscale</i> , 2012 , 4, 2839-2847	4.7	12
12	Mechanistic investigations on the adsorption of thiophene over Zn_3NiO_4 bimetallic oxide cluster. <i>Applied Surface Science</i> , 2012 , 258, 10148-10153	6.7	19
11	Effects of nonmetal element (B, C and Si) additives in Mg_2Ni hydrogen storage alloy: A first-principles study. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 6700-6713	6.7	14
10	Theoretical investigation of growth, stability, and electronic properties of beaded ZnO nanoclusters. <i>Journal of Materials Chemistry</i> , 2011 , 21, 16905		27
9	Field-Emission Mechanism of Island-Shaped Graphene/BN Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 9471-9476	3.8	14
8	Theoretical investigation of adsorption and dissociation of H_2 on $(\text{ZrO}_2)_n$ ($n=1-5$) clusters. <i>International Journal of Hydrogen Energy</i> , 2011 , 36, 9069-9078	6.7	17
7	First-Principles Study of Field Emission Properties of Graphene-ZnO Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 19284-19288	3.8	47
6	Molecular Dynamics Simulations of Silica Nanotube: Structural and Vibrational Properties Under Different Temperatures. <i>Chinese Journal of Chemical Physics</i> , 2010 , 23, 497-503	0.9	2

5	First-principles study of structural, electronic and vibrational properties of aluminum-doped silica nanotubes. <i>Chemical Physics Letters</i> , 2010 , 498, 172-177	2.5	12
4	A two-photon tandem black phosphorus quantum dot-sensitized BiVO ₄ photoanode for solar water splitting. <i>Energy and Environmental Science</i> ,	35.4	5
3	Pentagonal two-dimensional noble-metal dichalcogenide PdSSe for photocatalytic water splitting with pronounced optical absorption and ultrahigh anisotropic carrier mobility. <i>Journal of Materials Chemistry C</i> ,	7.1	5
2	Facet-induced coordination competition for highly ordered CsPbBr ₃ nanoplatelets with strong polarized emission. <i>Nano Research</i> ,1	10	2
1	Boosting Alkaline Hydrogen Evolution on Stoichiometric Molybdenum Carbonitride via an Interstitial Vacancy-Elimination Strategy. <i>Advanced Energy Materials</i> ,2200974	21.8	2