

Li-Min Liu

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176
papers

12,259
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107
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181
ext. papers

14,456
ext. citations

9.6
avg, IF

6.62
L-index

#	Paper	IF	Citations
176	Platinum single-atom and cluster catalysis of the hydrogen evolution reaction. <i>Nature Communications</i> , 2016 , 7, 13638	17.4	1085
175	Rational molecular passivation for high-performance perovskite light-emitting diodes. <i>Nature Photonics</i> , 2019 , 13, 418-424	33.9	638
174	A sulfur host based on titanium monoxide@carbon hollow spheres for advanced lithium-sulfur batteries. <i>Nature Communications</i> , 2016 , 7, 13065	17.4	511
173	Phenylalkylamine Passivation of Organolead Halide Perovskites Enabling High-Efficiency and Air-Stable Photovoltaic Cells. <i>Advanced Materials</i> , 2016 , 28, 9986-9992	24	425
172	Water at Interfaces. <i>Chemical Reviews</i> , 2016 , 116, 7698-726	68.1	388
171	Surface evolution of a PtPdAu electrocatalyst for stable oxygen reduction. <i>Nature Energy</i> , 2017 , 2,	62.3	233
170	Doping high-surface-area mesoporous TiO ₂ microspheres with carbonate for visible light hydrogen production. <i>Energy and Environmental Science</i> , 2014 , 7, 2592	35.4	232
169	Titania-water interactions: a review of theoretical studies. <i>Journal of Materials Chemistry</i> , 2010 , 20, 10319		228
168	Tuning defects in oxides at room temperature by lithium reduction. <i>Nature Communications</i> , 2018 , 9, 1302	17.4	225
167	A porous nitrogen and phosphorous dual doped graphene blocking layer for high performance LiS batteries. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 16670-16678	13	219
166	Iced photochemical reduction to synthesize atomically dispersed metals by suppressing nanocrystal growth. <i>Nature Communications</i> , 2017 , 8, 1490	17.4	219
165	First-Principles Study of Phosphorene and Graphene Heterostructure as Anode Materials for Rechargeable Li Batteries. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 5002-8	6.4	215
164	Hierarchical NiCo ₂ O ₄ nanosheets grown on Ni nanofoam as high-performance electrodes for supercapacitors. <i>Small</i> , 2015 , 11, 804-8	11	211
163	First-Principles Study of Lead Iodide Perovskite Tetragonal and Orthorhombic Phases for Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 19565-19571	3.8	196
162	Atomic layer deposited Pt-Ru dual-metal dimers and identifying their active sites for hydrogen evolution reaction. <i>Nature Communications</i> , 2019 , 10, 4936	17.4	186
161	Injection of oxygen vacancies in the bulk lattice of layered cathodes. <i>Nature Nanotechnology</i> , 2019 , 14, 602-608	28.7	180
160	Oxygen-doped boron nitride nanosheets with excellent performance in hydrogen storage. <i>Nano Energy</i> , 2014 , 6, 219-224	17.1	170

159	Structure and dynamics of liquid water on rutile TiO ₂ (110). <i>Physical Review B</i> , 2010 , 82,	3.3	162
158	First-principles study of polar Al/TiN(1 1 1) interfaces. <i>Acta Materialia</i> , 2004 , 52, 3681-3688	8.4	156
157	Dimension-dependent phase transition and magnetic properties of VS ₂ . <i>Journal of Materials Chemistry A</i> , 2013 , 1, 10821	13	154
156	Well-Dispersed Ruthenium in Mesoporous Crystal TiO as an Advanced Electrocatalyst for Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2018 , 140, 5719-5727	16.4	152
155	Uncovering the Veil of the Degradation in Perovskite CH ₃ NH ₃ PbI ₃ upon Humidity Exposure: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3289-3295	6.4	147
154	Two dimensional Dirac carbon allotropes from graphene. <i>Nanoscale</i> , 2014 , 6, 1113-8	7.7	147
153	Localized Excitation of Ti(3+) Ions in the Photoabsorption and Photocatalytic Activity of Reduced Rutile TiO ₂ . <i>Journal of the American Chemical Society</i> , 2015 , 137, 9146-52	16.4	139
152	Formation of Bi ₂ WO ₆ Bipyramids with Vacancy Pairs for Enhanced Solar-Driven Photoactivity. <i>Advanced Functional Materials</i> , 2015 , 25, 3726-3734	15.6	117
151	Pristine and defect-containing phosphorene as promising anode materials for rechargeable Li batteries. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 11246-11252	13	112
150	Optical properties and applications for MoS ₂ -Sb ₂ Te ₃ -MoS ₂ heterostructure materials. <i>Photonics Research</i> , 2018 , 6, 220	6	111
149	Self-hydrogenated shell promoting photocatalytic H evolution on anatase TiO. <i>Nature Communications</i> , 2018 , 9, 2752	17.4	111
148	The interaction between adsorbed OH and O ₂ on TiO ₂ surfaces. <i>Progress in Surface Science</i> , 2009 , 84, 155-176	6.6	111
147	Nanoporous Zn-doped Co ₃ O ₄ sheets with single-unit-cell-wide lateral surfaces for efficient oxygen evolution and water splitting. <i>Nano Energy</i> , 2018 , 44, 371-377	17.1	111
146	Tunable dipole and carrier mobility for a few layer Janus MoSSe structure. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 1693-1700	7.1	106
145	Combined Effects of Functional Groups, Lattice Defects, and Edges in the Infrared Spectra of Graphene Oxide. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 18167-18176	3.8	97
144	Thermal transport in graphyne nanoribbons. <i>Physical Review B</i> , 2012 , 85,	3.3	95
143	A highly stable bifunctional catalyst based on 3D Co(OH) ₂ @NCNTs@NF towards overall water-splitting. <i>Nano Energy</i> , 2018 , 47, 96-104	17.1	94
142	Growth and organization of an organic molecular monolayer on TiO ₂ : catechol on anatase (101). <i>Journal of the American Chemical Society</i> , 2011 , 133, 7816-23	16.4	93

141	New manifold two-dimensional single-layer structures of zinc-blende compounds. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 17971-17978	13	92
140	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 25854-61	3.6	90
139	R-graphyne: a new two-dimensional carbon allotrope with versatile Dirac-like point in nanoribbons. <i>Journal of Materials Chemistry A</i> , 2013 , 1, 5341	13	90
138	-60 °C solution synthesis of atomically dispersed cobalt electrocatalyst with superior performance. <i>Nature Communications</i> , 2019 , 10, 606	17.4	87
137	Defect Modulation of Z-Scheme TiO ₂ /Cu ₂ O Photocatalysts for Durable Water Splitting. <i>ACS Catalysis</i> , 2019 , 9, 8346-8354	13.1	86
136	The effect of water on the structural, electronic and photocatalytic properties of graphitic carbon nitride. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 3299-304	3.6	85
135	Diverse and tunable electronic structures of single-layer metal phosphorus trichalcogenides for photocatalytic water splitting. <i>Journal of Chemical Physics</i> , 2014 , 140, 054707	3.9	76
134	Excess electrons in reduced rutile and anatase TiO ₂ . <i>Surface Science Reports</i> , 2018 , 73, 58-82	12.9	75
133	New Insights into Defect-Mediated Heterostructures for Photoelectrochemical Water Splitting. <i>Advanced Energy Materials</i> , 2016 , 6, 1502268	21.8	75
132	Structures, stabilities, and electronic properties of defects in monolayer black phosphorus. <i>Scientific Reports</i> , 2015 , 5, 10848	4.9	72
131	Enhanced thermal decomposition of nitromethane on functionalized graphene sheets: ab initio molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , 2012 , 134, 19011-6	16.4	72
130	Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 15389-15395	13	71
129	Modulating the atomic and electronic structures through alloying and heterostructure of single-layer MoS ₂ . <i>Journal of Materials Chemistry A</i> , 2014 , 2, 2101-2109	13	69
128	Single-layer Group-IVB nitride halides as promising photocatalysts. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 6755	13	69
127	Ball-milling synthesis of ZnO@sulphur/carbon nanotubes and Ni(OH) ₂ @sulphur/carbon nanotubes composites for high-performance lithium-sulphur batteries. <i>Electrochimica Acta</i> , 2016 , 196, 369-376	6.7	68
126	Multi-electric field modulation for photocatalytic oxygen evolution: Enhanced charge separation by coupling oxygen vacancies with faceted heterostructures. <i>Nano Energy</i> , 2018 , 51, 764-773	17.1	68
125	Ultrathin NiCo ₂ O ₄ nanosheets grown on three-dimensional interwoven nitrogen-doped carbon nanotubes as binder-free electrodes for high-performance supercapacitors. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 15331-15338	13	68
124	Porous BN for hydrogen generation and storage. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 9632-9637	13	65

123	The intrinsic mechanism of methane oxidation under explosion condition: A combined ReaxFF and DFT study. <i>Fuel</i> , 2014 , 124, 85-90	7.1	65
122	Surface energy and surface proton order of ice Ih. <i>Physical Review Letters</i> , 2008 , 101, 155703	7.4	65
121	Band-Gap States of TiO ₂ (110): Major Contribution from Surface Defects. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3839-3844	6.4	62
120	EMnO ₂ as a cathode material for lithium ion batteries from first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 9075-83	3.6	62
119	Structures and Electronic Properties of Different CH ₃ NH ₃ PbI ₃ /TiO ₂ Interface: A First-Principles Study. <i>Scientific Reports</i> , 2016 , 6, 20131	4.9	60
118	Potential Application of Metal Dichalcogenides Double-Layered Heterostructures as Anode Materials for Li-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 4779-4788	3.8	59
117	Melting the ice: on the relation between melting temperature and size for nanoscale ice crystals. <i>ACS Nano</i> , 2011 , 5, 4562-9	16.7	59
116	Enhanced Thermoelectric Properties of Cu ₂ SnSe ₃ by (Ag,In)-Co-Doping. <i>Advanced Functional Materials</i> , 2016 , 26, 6025-6032	15.6	59
115	From melamine-resorcinol-formaldehyde to nitrogen-doped carbon xerogels with micro- and meso-pores for lithium batteries. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 14429-14438	13	58
114	Three-dimensional hierarchical interwoven nitrogen-doped carbon nanotubes/CoxNi _{1-x} -layered double hydroxides ultrathin nanosheets for high-performance supercapacitors. <i>Electrochimica Acta</i> , 2016 , 203, 21-29	6.7	58
113	Synergy between Ion Migration and Charge Carrier Recombination in Metal-Halide Perovskites. <i>Journal of the American Chemical Society</i> , 2020 , 142, 3060-3068	16.4	55
112	Role of Methylammonium Orientation in Ion Diffusion and Current-Voltage Hysteresis in the CH ₃ NH ₃ PbI ₃ Perovskite. <i>ACS Energy Letters</i> , 2017 , 2, 1997-2004	20.1	55
111	An electron injection promoted highly efficient electrocatalyst of FeNi ₃ @GR@Fe-NiOOH for oxygen evolution and rechargeable metal-air batteries. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 7762-7771	13	55
110	Ultra-small B ₂ O ₃ nanocrystals grown in situ on highly porous carbon microtubes for lithium-iodine and lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 8541-8547	13	54
109	Multifunctional Nitrogen-Doped Loofah Sponge Carbon Blocking Layer for High-Performance Rechargeable Lithium Batteries. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 15991-6001	9.5	52
108	Two-Dimensional Superlattice: Modulation of Band Gaps in Graphene-Based Monolayer Carbon Superlattices. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3373-3378	6.4	52
107	Coverage Dependence of Methanol Dissociation on TiO(110). <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3327-3334	6.4	51
106	Hierarchical three-dimensional NiCo ₂ O ₄ nanoneedle arrays supported on Ni foam for high-performance supercapacitors. <i>RSC Advances</i> , 2015 , 5, 25304-25311	3.7	51

105	An ab initio study of TiS ₃ : a promising electrode material for rechargeable Li and Na ion batteries. <i>RSC Advances</i> , 2015 , 5, 21455-21463	3.7	49
104	CO ₂ Capture and Conversion on Rutile TiO ₂ (110) in the Water Environment: Insight by First-Principles Calculations. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2538-45	6.4	49
103	First-Principles Study of Novel Two-Dimensional (CHNH)PbX Perovskites for Solar Cell Absorbers. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 876-883	6.4	46
102	Valence oscillation and dynamic active sites in monolayer NiCo hydroxides for water oxidation. <i>Nature Catalysis</i> , 2021 , 4, 1050-1058	36.5	46
101	Spatial separation of photo-generated electron-hole pairs in BiOBr/BiOI bilayer to facilitate water splitting. <i>Scientific Reports</i> , 2016 , 6, 32764	4.9	44
100	Interfacial water: a first principles molecular dynamics study of a nanoscale water film on salt. <i>Journal of Chemical Physics</i> , 2009 , 130, 234702	3.9	44
99	Boosting photoelectrochemical activities of heterostructured photoanodes through interfacial modulation of oxygen vacancies. <i>Nano Energy</i> , 2017 , 35, 290-298	17.1	43
98	Effect of surface composition on electronic properties of methylammonium lead iodide perovskite. <i>Journal of Materiomics</i> , 2015 , 1, 213-220	6.7	42
97	Tailor-made metal-nitrogen-carbon bifunctional electrocatalysts for rechargeable Zn-air batteries via controllable MOF units. <i>Energy Storage Materials</i> , 2019 , 17, 46-61	19.4	42
96	Effect of Surface Structure on the Photoreactivity of TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2015 , 119, 6121-6127	3.8	41
95	Long Carrier Lifetimes in PbI ₂ -Rich Perovskites Rationalized by Ab Initio Nonadiabatic Molecular Dynamics. <i>ACS Energy Letters</i> , 2018 , 3, 1868-1874	20.1	41
94	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 13162-6	3.6	41
93	Visible-light induced photocatalytic activity of electrospun-TiO ₂ in arsenic(III) oxidation. <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 511-8	9.5	39
92	High performance NiO nanosheets anchored on three-dimensional nitrogen-doped carbon nanotubes as a binder-free anode for lithium ion batteries. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 10940-10947	13	39
91	Enhanced optical absorption via cation doping hybrid lead iodine perovskites. <i>Scientific Reports</i> , 2017 , 7, 7843	4.9	39
90	The stability and electronic properties of novel three-dimensional graphene-MoS ₂ hybrid structure. <i>Scientific Reports</i> , 2014 , 4, 7007	4.9	37
89	Phosphorene ribbons as anode materials with superhigh rate and large capacity for Li-ion batteries. <i>Journal of Power Sources</i> , 2016 , 302, 215-222	8.9	37
88	Tunable electronic and magnetic properties of WS ₂ nanoribbons. <i>Journal of Applied Physics</i> , 2013 , 114, 093710	2.5	37

87	Engineering the Low Coordinated Pt Single Atom to Achieve the Superior Electrocatalytic Performance toward Oxygen Reduction. <i>Small</i> , 2020 , 16, e2003096	11	36
86	Dynamic Responses and Initial Decomposition under Shock Loading: A DFTB Calculation Combined with MSST Method for HMX with Molecular Vacancy. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 10673-814	3.4	35
85	Modulating the phase transition between metallic and semiconducting single-layer MoS2 and WS2 through size effects. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 1099-105	3.6	35
84	Surface energy and surface proton order of the ice Ih basal and prism surfaces. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 074209	1.8	35
83	Thiolate-Mediated Photoinduced Synthesis of Ultrafine Ag S Quantum Dots from Silver Nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 14952-14957	16.4	33
82	Band gap engineering of FeS2 under biaxial strain: a first principles study. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 24466-72	3.6	31
81	Substitution Boosts Charge Separation for High Solar-Driven Photocatalytic Performance. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 26783-26793	9.5	30
80	Porous structure design of carbon xerogels for advanced supercapacitor. <i>Applied Energy</i> , 2015 , 153, 32-40.	4.7	29
79	Ultrahigh capacitive performance of three-dimensional electrode nanomaterials based on MnO2 nanocrystallines induced by doping Au through scale channels. <i>Nano Energy</i> , 2016 , 21, 39-50	17.1	29
78	High carrier mobility of few-layer PbX (X = S, Se, Te). <i>Journal of Materials Chemistry C</i> , 2015 , 3, 6284-6290.	7.1	29
77	The Effect of Excess Electron and hole on CO2 Adsorption and Activation on Rutile (110) surface. <i>Scientific Reports</i> , 2016 , 6, 23298	4.9	29
76	Reply to Comment on 'Structure and dynamics of liquid water on rutile TiO2(110)' <i>Physical Review B</i> , 2012 , 85,	3.3	28
75	Improved Electrocatalytic Performance in Overall Water Splitting with Rational Design of Hierarchical Co3O4@NiFe Layered Double Hydroxide Core-Shell Nanostructure. <i>ChemElectroChem</i> , 2018 , 5, 1357-1363	4.3	27
74	Unusual Li-Ion Transfer Mechanism in Liquid Electrolytes: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4795-4801	6.4	27
73	First-Principles Study of Methanol Oxidation into Methyl Formate on Rutile TiO2(110). <i>Journal of Physical Chemistry C</i> , 2014 , 118, 19859-19868	3.8	27
72	Effect of Single-Atom Cocatalysts on the Activity of Faceted TiO Photocatalysts. <i>Langmuir</i> , 2019 , 35, 391-397	4	27
71	Electronic structure and photoabsorption of Ti ions in reduced anatase and rutile TiO. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 17658-17665	3.6	27
70	Wurtzite-type CuInSe2 for high-performance solar cell absorber: ab initio exploration of the new phase structure. <i>Journal of Materials Chemistry</i> , 2012 , 22, 21662		26

69	Tuning band gaps and optical absorption of BiOCl through doping and strain: insight from DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 20968-20973	3.6	25
68	Defects, Adsorbates, and Photoactivity of Rutile TiO (110): Insight by First-Principles Calculations. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5281-5287	6.4	25
67	Ice Melting to Release Reactants in Solution Syntheses. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 3354-3359	16.4	24
66	The oxygen vacancy in Li-ion battery cathode materials. <i>Nanoscale Horizons</i> , 2020 , 5, 1453-1466	10.8	24
65	Efficient design principle for interfacial charge separation in hydrogen-intercalated nonstoichiometric oxides. <i>Nano Energy</i> , 2018 , 53, 887-897	17.1	24
64	Janus MoSSe Nanotubes: Tunable Band Gap and Excellent Optical Properties for Surface Photocatalysis. <i>Advanced Theory and Simulations</i> , 2018 , 1, 1800082	3.5	23
63	Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. <i>Journal of Applied Physics</i> , 2014 , 115, 093504	2.5	23
62	A first-principles study of lithium-decorated hybrid boron nitride and graphene domains for hydrogen storage. <i>Journal of Chemical Physics</i> , 2014 , 141, 084711	3.9	22
61	Robust vanadium pentoxide electrodes for sodium and calcium ion batteries: thermodynamic and diffusion mechanical insights. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 12516-12525	13	22
60	Structural resolution of inorganic nanotubes with complex stoichiometry. <i>Nature Communications</i> , 2018 , 9, 2033	17.4	22
59	New insights into interfacial photocharge transfer in TiO ₂ /C ₃ N ₄ heterostructures: effects of facets and defects. <i>New Journal of Chemistry</i> , 2019 , 43, 4511-4517	3.6	21
58	Porous CoP nanosheet arrays grown on nickel foam as an excellent and stable catalyst for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 26995-27003	6.7	20
57	The role of the defect on the adsorption and dissociation of water on graphitic carbon nitride. <i>Applied Surface Science</i> , 2015 , 358, 363-369	6.7	20
56	Water Film Adsorbed on the Al ₂ O ₃ (0001) Surface: Structural Properties and Dynamical Behaviors from First-Principles Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 5398-5409	2.8	20
55	The microstructure, stability, and elastic properties of 14H long-period stacking-ordered phase in MgZn alloys: a first-principles study. <i>Journal of Materials Science</i> , 2014 , 49, 737-748	4.3	19
54	Tunable band gap and magnetism of the two-dimensional nickel hydroxide. <i>RSC Advances</i> , 2015 , 5, 77154-77158	3.7	18
53	Increasing the band gap of FeS ₂ by alloying with Zn and applying biaxial strain: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2015 , 629, 43-48	5.7	18
52	Tuning the electronic properties of half- and full-hydrogenated germanene by chlorination and hydroxylation: A first-principles study. <i>Computational Materials Science</i> , 2014 , 92, 244-252	3.2	17

51	The predominant role of Zn ₆ Y ₉ cluster in the long period stacking order structures of Mg ₂ Zn ₃ alloys: a first-principles study. <i>Journal of Materials Science</i> , 2013 , 48, 1407-1412	4.3	17
50	Two-dimensional square-pyramidal VO ₂ with tunable electronic properties. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 3189-3197	7.1	16
49	New Insight of Pyrrole-Like Nitrogen for Boosting Hydrogen Evolution Activity and Stability of Pt Single Atoms. <i>Small</i> , 2021 , 17, e2004453	11	15
48	Novel monolayer pyrite FeS ₂ with atomic-thickness for magnetic devices. <i>Computational Materials Science</i> , 2015 , 101, 255-259	3.2	14
47	Theoretical study on the composition location of the best glass formers in Cu-Zr amorphous alloys. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 806-14	2.8	14
46	Amorphous Domains in Black Titanium Dioxide. <i>Advanced Materials</i> , 2021 , 33, e2100407	24	14
45	How Hole Injection Accelerates Both Ion Migration and Nonradiative Recombination in Metal Halide Perovskites.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	14
44	Cu ₂ ZnSnS ₄ Nanocrystals as Highly Active and Stable Electrocatalysts for the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 24265-24270	3.8	13
43	Atomic structure and electronic properties of folded graphene nanoribbons: A first-principles study. <i>Journal of Applied Physics</i> , 2013 , 113, 173506	2.5	13
42	Versatile electronic properties and exotic edge states of single-layer tetragonal silicon carbides. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 11211-6	3.6	12
41	Solid wetting-layers in inorganic nano-reactors: the water in imogolite nanotube case. <i>Nanoscale Advances</i> , 2020 , 2, 1869-1877	5.1	11
40	A strain or electric field induced direct bandgap in ultrathin silicon film and its application in photovoltaics or photocatalysis. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 7156-62	3.6	11
39	Effect of water on gas explosions: combined ReaxFF and ab initio MD calculations. <i>RSC Advances</i> , 2014 , 4, 35048	3.7	11
38	Direct observation of multiple rotational stacking faults coexisting in freestanding bilayer MoS ₂ . <i>Scientific Reports</i> , 2017 , 7, 8323	4.9	11
37	Periodic continuum solvation model integrated with first-principles calculations for solid surfaces. <i>Progress in Natural Science: Materials International</i> , 2017 , 27, 283-288	3.6	10
36	Inherent Simple Cubic Lattice Being Responsible for Ultrafast Solid-Phase Change of GeSbTe. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2560-2564	6.4	10
35	Subnano Ruthenium Species Anchored on Tin Dioxide Surface for Efficient Alkaline Hydrogen Evolution Reaction. <i>Cell Reports Physical Science</i> , 2020 , 1, 100026	6.1	10
34	Electrocatalysis enhancement of iron-based catalysts induced by synergy of methanol and oxygen-containing groups. <i>Nano Energy</i> , 2016 , 21, 265-275	17.1	10

33	Electric field and strain tunable electronic structures in monolayer Black Phosphorus. <i>Computational Materials Science</i> , 2016 , 112, 297-303	3.2	10
32	A low-surface energy carbon allotrope: the case for bcc-C6. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 14083-7	3.6	9
31	Two-dimensional Ni(OH) ₂ -XS ₂ (X = Mo and W) heterostructures. <i>2D Materials</i> , 2015 , 2, 034014	5.9	9
30	Water-Hydrogen-Polaron Coupling at Anatase TiO(101) Surfaces: A Hybrid Density Functional Theory Study. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 4317-4325	6.4	9
29	Electronic and magnetism properties of two-dimensional stacked nickel hydroxides and nitrides. <i>Scientific Reports</i> , 2015 , 5, 11656	4.9	8
28	Bipolar doping of double-layer graphene vertical heterostructures with hydrogenated boron nitride. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 11692-9	3.6	8
27	Activity and selectivity of CO photoreduction on catalytic materials. <i>Dalton Transactions</i> , 2020 , 49, 12918-12928	4.3	8
26	Effect of water on the effective Goldschmidt tolerance factor and photoelectric conversion efficiency of organic-inorganic perovskite: insights from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 14955-14960	3.6	6
25	Space-confined creation of nanoframes in situ on reduced graphene oxide. <i>Small</i> , 2015 , 11, 1512-8	11	6
24	Self-Induced Strain in 2D Chalcogenide Nanocrystals with Enhanced Photoelectrochemical Responsivity. <i>Chemistry of Materials</i> , 2020 , 32, 2774-2781	9.6	6
23	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO ₃ from First Principles. <i>ACS Catalysis</i> , 2019 , 9, 10528-10535	13.1	6
22	Recent advances in low-dimensional Janus materials: theoretical and simulation perspectives. <i>Materials Advances</i> ,	3.3	6
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