Li-Min Liu

List of Publications by Year
in descending order

179	16,757	13827 67	15683 125
papers	citations	h-index	g-index

181	181	181	23100
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Platinum single-atom and cluster catalysis of the hydrogen evolution reaction. Nature Communications, 2016, 7, 13638.	5.8	1,521
2	Rational molecular passivation for high-performance perovskite light-emitting diodes. Nature Photonics, 2019, 13, 418-424.	15.6	970
3	A sulfur host based on titanium monoxide@carbon hollow spheres for advanced lithiumâ€“sulfur batteries. Nature Communications, 2016, 7, 13065.	5.8	590
4	Water at Interfaces. Chemical Reviews, 2016, 116, 7698-7726.	23.0	536
5	Phenylalkylamine Passivation of Organolead Halide Perovskites Enabling Highâ€Efficiency and Airâ€Stable Photovoltaic Cells. Advanced Materials, 2016, 28, 9986-9992.	11.1	532
6	Tuning defects in oxides at roomÂtemperature by lithium reduction. Nature Communications, 2018, 9, 1302.	5.8	428
7	Atomic layer deposited Pt-Ru dual-metal dimers and identifying their active sites for hydrogen evolution reaction. Nature Communications, 2019, 10, 4936.	5.8	371
8	Iced photochemical reduction to synthesize atomically dispersed metals by suppressing nanocrystal growth. Nature Communications, 2017, 8, 1490.	5.8	322
9	Injection of oxygen vacancies in the bulk lattice of layered cathodes. Nature Nanotechnology, 2019, 14, 602-608.	15.6	321
10	Surface evolution of a Ptâ€“Pdâ€“Au electrocatalyst for stable oxygen reduction. Nature Energy, 2017, 2, .	19.8	302
11	First-Principles Study of Phosphorene and Graphene Heterostructure as Anode Materials for Rechargeable Li Batteries. Journal of Physical Chemistry Letters, 2015, 6, 5002-5008.	2.1	274
12	Valence oscillation and dynamic active sites in monolayer NiCo hydroxides for water oxidation. Nature Catalysis, 2021, 4, 1050-1058.	16.1	272
13	Titania-water interactions: a review of theoretical studies. Journal of Materials Chemistry, 2010, 20, 10319.	6.7	255
14	Doping high-surface-area mesoporous TiO₂microspheres with carbonate for visible light hydrogen production. Energy and Environmental Science, 2014, 7, 2592.	15.6	253
15	A porous nitrogen and phosphorous dual doped graphene blocking layer for high performance Liâ€“S batteries. Journal of Materials Chemistry A, 2015, 3, 16670-16678.	5.2	241
16	Hierarchical NiCo₂O₄Nanosheets Grown on Ni Nanofoam as High-Performance Electrodes for Supercapacitors. Small, 2015, 11, 804-808.	5.2	232
17	Well-Dispersed Ruthenium in Mesoporous Crystal TiO₂ as an Advanced Electrocatalyst for Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 5719-5727.	6.6	224
18	First-Principles Study of Lead Iodide Perovskite Tetragonal and Orthorhombic Phases for Photovoltaics. Journal of Physical Chemistry C, 2014, 118, 19565-19571.	1.5	220

#	Article	IF	Citations
19	Oxygen-doped boron nitride nanosheets with excellent performance in hydrogen storage. Nano Energy, 2014, 6, 219-224.	8.2	210
20	Two dimensional Dirac carbon allotropes from graphene. Nanoscale, 2014, 6, 1113-1118.	2.8	198
21	First-principles study of polar Al/TiN(1 1 1) interfaces. Acta Materialia, 2004, 52, 3681-3688.	3.8	191
22	Dimension-dependent phase transition and magnetic properties of VS2. Journal of Materials Chemistry A, 2013, 1, 10821.	5.2	183
23	Structure and dynamics of liquid water on rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2010, 82, .	1.1	182
24	Self-hydrogenated shell promoting photocatalytic H2 evolution on anatase TiO2. Nature Communications, 2018, 9, 2752.	5.8	178
25	Uncovering the Veil of the Degradation in Perovskite CH₃NH₃PbI₃ upon Humidity Exposure: A First-Principles Study. Journal of Physical Chemistry Letters, 2015, 6, 3289-3295.	2.1	171
26	Localized Excitation of Ti³⁺ Ions in the Photoabsorption and Photocatalytic Activity of Reduced Rutile TiO₂. Journal of the American Chemical Society, 2015, 137, 9146-9152.	6.6	168
27	Tunable dipole and carrier mobility for a few layer Janus MoSSe structure. Journal of Materials Chemistry C, 2018, 6, 1693-1700.	2.7	164
28	Formation of Bi₂WO₆ Bipyramids with Vacancy Pairs for Enhanced Solarâ€Driven Photoactivity. Advanced Functional Materials, 2015, 25, 3726-3734.	7.8	155
29	Defect Modulation of Z-Scheme TiO₂/Cu₂O Photocatalysts for Durable Water Splitting. ACS Catalysis, 2019, 9, 8346-8354.	5.5	146
30	Optical properties and applications for MoS₂-Sb₂Te₃-MoS₂heterostructure materials. Photonics Research, 2018, 6, 220.	3.4	141
31	Nanoporous Zn-doped Co3O4 sheets with single-unit-cell-wide lateral surfaces for efficient oxygen evolution and water splitting. Nano Energy, 2018, 44, 371-377.	8.2	138
32	Pristine and defect-containing phosphorene as promising anode materials for rechargeable Li batteries. Journal of Materials Chemistry A, 2015, 3, 11246-11252.	5.2	136
33	Combined Effects of Functional Groups, Lattice Defects, and Edges in the Infrared Spectra of Graphene Oxide. Journal of Physical Chemistry C, 2015, 119, 18167-18176.	1.5	134
34	The interaction between adsorbed OH and O2 on TiO2 surfaces. Progress in Surface Science, 2009, 84, 155-176.	3.8	126
35	A highly stable bifunctional catalyst based on 3D Co(OH)2@NCNTs@NF towards overall water-splitting. Nano Energy, 2018, 47, 96-104.	8.2	121
36	â^'60â€‰Â°C solution synthesis of atomically dispersed cobalt electrocatalyst with superior performance. Nature Communications, 2019, 10, 606.	5.8	121

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37	R-graphyne: a new two-dimensional carbon allotrope with versatile Dirac-like point in nanoribbons. Journal of Materials Chemistry A, 2013, 1, 5341.	5.2	118
38	Realizing Two-Electron Transfer in Ni(OH)₂ Nanosheets for Energy Storage. Journal of the American Chemical Society, 2022, 144, 8969-8976.	6.6	116
39	Engineering the Low Coordinated Pt Single Atom to Achieve the Superior Electrocatalytic Performance toward Oxygen Reduction. Small, 2020, 16, e2003096.	5.2	110
40	New manifold two-dimensional single-layer structures of zinc-blende compounds. Journal of Materials Chemistry A, 2014, 2, 17971-17978.	5.2	107
41	Growth and Organization of an Organic Molecular Monolayer on TiO₂: Catechol on Anatase (101). Journal of the American Chemical Society, 2011, 133, 7816-7823.	6.6	106
42	Excess electrons in reduced rutile and anatase TiO2. Surface Science Reports, 2018, 73, 58-82.	3.8	106
43	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. Physical Chemistry Chemical Physics, 2014, 16, 25854-25861.	1.3	105
44	Thermal transport in graphyne nanoribbons. Physical Review B, 2012, 85, .	1.1	103
45	Diverse and tunable electronic structures of single-layer metal phosphorus trichalcogenides for photocatalytic water splitting. Journal of Chemical Physics, 2014, 140, 054707.	1.2	99
46	The effect of water on the structural, electronic and photocatalytic properties of graphitic carbon nitride. Physical Chemistry Chemical Physics, 2014, 16, 3299.	1.3	97
47	New Insights into Defectâ€Mediated Heterostructures for Photoelectrochemical Water Splitting. Advanced Energy Materials, 2016, 6, 1502268.	10.2	95
48	Modulating the atomic and electronic structures through alloying and heterostructure of single-layer MoS₂. Journal of Materials Chemistry A, 2014, 2, 2101-2109.	5.2	92
49	Potential Application of Metal Dichalcogenides Double-Layered Heterostructures as Anode Materials for Li-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 4779-4788.	1.5	92
50	Synergy between Ion Migration and Charge Carrier Recombination in Metal-Halide Perovskites. Journal of the American Chemical Society, 2020, 142, 3060-3068.	6.6	91
51	Single-layer Group-IVB nitride halides as promising photocatalysts. Journal of Materials Chemistry A, 2014, 2, 6755.	5.2	90
52	The intrinsic mechanism of methane oxidation under explosion condition: A combined ReaxFF and DFT study. Fuel, 2014, 124, 85-90.	3.4	90
53	Structures, stabilities and electronic properties of defects in monolayer black phosphorus. Scientific Reports, 2015, 5, 10848.	1.6	90
54	Multi-electric field modulation for photocatalytic oxygen evolution: Enhanced charge separation by coupling oxygen vacancies with faceted heterostructures. Nano Energy, 2018, 51, 764-773.	8.2	88

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55	Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion. Journal of Materials Chemistry A, 2014, 2, 15389-15395.	5.2	87
56	Enhanced Thermal Decomposition of Nitromethane on Functionalized Graphene Sheets: Ab Initio Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 19011-19016.	6.6	83
57	Porous BN for hydrogen generation and storage. Journal of Materials Chemistry A, 2015, 3, 9632-9637.	5.2	83
58	Enhanced Thermoelectric Properties of Cu₂SnSe₃ by (Ag,In)â€Coâ€Doping. Advanced Functional Materials, 2016, 26, 6025-6032.	7.8	82
59	Ball-milling synthesis of ZnO@sulphur/carbon nanotubes and Ni(OH)2@sulphur/carbon nanotubes composites for high-performance lithium-sulphur batteries. Electrochimica Acta, 2016, 196, 369-376.	2.6	77
60	The oxygen vacancy in Li-ion battery cathode materials. Nanoscale Horizons, 2020, 5, 1453-1466.	4.1	77
61	Band-Gap States of TiO₂(110): Major Contribution from Surface Defects. Journal of Physical Chemistry Letters, 2013, 4, 3839-3844.	2.1	76
62	Ultrathin NiCo₂O₄nanosheets grown on three-dimensional interwoven nitrogen-doped carbon nanotubes as binder-free electrodes for high-performance supercapacitors. Journal of Materials Chemistry A, 2015, 3, 15331-15338.	5.2	76
63	Î²-MnO2 as a cathode material for lithium ion batteries from first principles calculations. Physical Chemistry Chemical Physics, 2013, 15, 9075.	1.3	74
64	Ultra-small B₂O₃ nanocrystals grown in situ on highly porous carbon microtubes for lithiumâ€“iodine and lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2016, 4, 8541-8547.	5.2	74
65	Surface Energy and Surface Proton Order of Ice<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="normal">I</mml:mi><mml:mi>h</mml:mi></mml:math>. Physical Review Letters, 2008, 101, 155703.	2.9	70
66	An electron injection promoted highly efficient electrocatalyst of FeNi₃@GR@Fe-NiOOH for oxygen evolution and rechargeable metalâ€“air batteries. Journal of Materials Chemistry A, 2016, 4, 7762-7771.	5.2	70
67	Tailor-made metal-nitrogen-carbon bifunctional electrocatalysts for rechargeable Zn-air batteries via controllable MOF units. Energy Storage Materials, 2019, 17, 46-61.	9.5	70
68	Structures and Electronic Properties of Different CH3NH3PbI3/TiO2 Interface: A First-Principles Study. Scientific Reports, 2016, 6, 20131.	1.6	69
69	Role of Methylammonium Orientation in Ion Diffusion and Currentâ€“Voltage Hysteresis in the CH₃NH₃PbI₃ Perovskite. ACS Energy Letters, 2017, 2, 1997-2004.	8.8	68
70	Hierarchical three-dimensional NiCo₂O₄ nanoneedle arrays supported on Ni foam for high-performance supercapacitors. RSC Advances, 2015, 5, 25304-25311.	1.7	67
71	From melamineâ€“resorcinolâ€“formaldehyde to nitrogen-doped carbon xerogels with micro- and meso-pores for lithium batteries. Journal of Materials Chemistry A, 2014, 2, 14429-14438.	5.2	66
72	Melting the Ice: On the Relation between Melting Temperature and Size for Nanoscale Ice Crystals. ACS Nano, 2011, 5, 4562-4569.	7.3	65

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73	Multifunctional Nitrogen-Doped Loofah Sponge Carbon Blocking Layer for High-Performance Rechargeable Lithium Batteries. ACS Applied Materials & Interfaces, 2016, 8, 15991-16001.	4.0	64
74	Three-dimensional hierarchical interwoven nitrogen-doped carbon nanotubes/CoxNi1-x-layered double hydroxides ultrathin nanosheets for high-performance supercapacitors. Electrochimica Acta, 2016, 203, 21-29.	2.6	63
75	Coverage Dependence of Methanol Dissociation on TiO₂(110). Journal of Physical Chemistry Letters, 2015, 6, 3327-3334.	2.1	62
76	First-Principles Study of Novel Two-Dimensional (C₄H₉NH₃)₂PbX₄ Perovskites for Solar Cell Absorbers. Journal of Physical Chemistry Letters, 2017, 8, 876-883.	2.1	61
77	Enhanced optical absorption via cation doping hybrid lead iodine perovskites. Scientific Reports, 2017, 7, 7843.	1.6	61
78	Two-Dimensional Superlattice: Modulation of Band Gaps in Graphene-Based Monolayer Carbon Superlattices. Journal of Physical Chemistry Letters, 2012, 3, 3373-3378.	2.1	60
79	CO₂ Capture and Conversion on Rutile TiO₂(110) in the Water Environment: Insight by First-Principles Calculations. Journal of Physical Chemistry Letters, 2015, 6, 2538-2545.	2.1	60
80	Boosting photoelectrochemical activities of heterostructured photoanodes through interfacial modulation of oxygen vacancies. Nano Energy, 2017, 35, 290-298.	8.2	59
81	An ab initio study of TiS₃: a promising electrode material for rechargeable Li and Na ion batteries. RSC Advances, 2015, 5, 21455-21463.	1.7	58
82	High performance NiO nanosheets anchored on three-dimensional nitrogen-doped carbon nanotubes as a binder-free anode for lithium ion batteries. Journal of Materials Chemistry A, 2016, 4, 10940-10947.	5.2	55
83	Long Carrier Lifetimes in PbI₂-Rich Perovskites Rationalized by Ab Initio Nonadiabatic Molecular Dynamics. ACS Energy Letters, 2018, 3, 1868-1874.	8.8	54
84	Effect of Single-Atom Cocatalysts on the Activity of Faceted TiO₂ Photocatalysts. Langmuir, 2019, 35, 391-397.	1.6	54
85	Spatial separation of photo-generated electron-hole pairs in BiOBr/BiOI bilayer to facilitate water splitting. Scientific Reports, 2016, 6, 32764.	1.6	53
86	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 13162.	1.3	51
87	Dynamic Responses and Initial Decomposition under Shock Loading: A DFTB Calculation Combined with MSST Method for Î²-HMX with Molecular Vacancy. Journal of Physical Chemistry B, 2015, 119, 10673-10681.	1.2	49
88	Effect of surface composition on electronic properties of methylammonium lead iodide perovskite. Journal of Materiomics, 2015, 1, 213-220.	2.8	49
89	Tunable electronic and magnetic properties of WS2 nanoribbons. Journal of Applied Physics, 2013, 114, .	1.1	48
90	Phosphorene ribbons as anode materials with superhigh rate and large capacity for Li-ion batteries. Journal of Power Sources, 2016, 302, 215-222.	4.0	46

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91	Interfacial water: A first principles molecular dynamics study of a nanoscale water film on salt. Journal of Chemical Physics, 2009, 130, 234702.	1.2	45
92	The stability and electronic properties of novel three-dimensional graphene-MoS2 hybrid structure. Scientific Reports, 2014, 4, 7007.	1.6	45
93	Porous structure design of carbon xerogels for advanced supercapacitor. Applied Energy, 2015, 153, 32-40.	5.1	44
94	Effect of Surface Structure on the Photoreactivity of TiO₂. Journal of Physical Chemistry C, 2015, 119, 6121-6127.	1.5	43
95	Visible-Light Induced Photocatalytic Activity of Electrospun-TiO₂ in Arsenic(III) Oxidation. ACS Applied Materials & Interfaces, 2015, 7, 511-518.	4.0	42
96	Facet-Regulating Local Coordination of Dual-Atom Cocatalyzed TiO₂ for Photocatalytic Water Splitting. ACS Catalysis, 2021, 11, 14669-14676.	5.5	42
97	High carrier mobility of few-layer PbX (X = S, Se, Te). Journal of Materials Chemistry C, 2015, 3, 6284-6290.	2.7	41
98	Surface energy and surface proton order of the ice Ih basal and prism surfaces. Journal of Physics Condensed Matter, 2010, 22, 074209.	0.7	40
99	Substitution Boosts Charge Separation for High Solar-Driven Photocatalytic Performance. ACS Applied Materials & Interfaces, 2016, 8, 26783-26793.	4.0	39
100	Unusual Li-Ion Transfer Mechanism in Liquid Electrolytes: A First-Principles Study. Journal of Physical Chemistry Letters, 2016, 7, 4795-4801.	2.1	39
101	Band gap engineering of FeS₂ under biaxial strain: a first principles study. Physical Chemistry Chemical Physics, 2014, 16, 24466-24472.	1.3	38
102	Modulating the phase transition between metallic and semiconducting single-layer MoS₂ and WS₂ through size effects. Physical Chemistry Chemical Physics, 2015, 17, 1099-1105.	1.3	38
103	The Effect of Excess Electron and hole on CO2 Adsorption and Activation on Rutile (110) surface. Scientific Reports, 2016, 6, 23298.	1.6	38
104	Thiolateâ€Mediated Photoinduced Synthesis of Ultrafine Ag₂S Quantum Dots from Silver Nanoparticles. Angewandte Chemie - International Edition, 2016, 55, 14952-14957.	7.2	38
105	Electronic structure and photoabsorption of Ti³⁺ ions in reduced anatase and rutile TiO₂. Physical Chemistry Chemical Physics, 2018, 20, 17658-17665.	1.3	38
106	New Insight of Pyroleâ€Like Nitrogen for Boosting Hydrogen Evolution Activity and Stability of Pt Single Atoms. Small, 2021, 17, e2004453.	5.2	38
107	Recent advances in low-dimensional Janus materials: theoretical and simulation perspectives. Materials Advances, 2021, 2, 7543-7558.	2.6	38
108	Ice Melting to Release Reactants in Solution Syntheses. Angewandte Chemie - International Edition, 2018, 57, 3354-3359.	7.2	36

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109	Amorphous Domains in Black Titanium Dioxide. Advanced Materials, 2021, 33, e2100407.	11.1	36
110	Janus MoSSe Nanotubes: Tunable Band Gap and Excellent Optical Properties for Surface Photocatalysis. Advanced Theory and Simulations, 2018, 1, 1800082.	1.3	35
111	Tuning band gaps and optical absorption of BiOCl through doping and strain: insight form DFT calculations. Physical Chemistry Chemical Physics, 2017, 19, 20968-20973.	1.3	34
112	Improved Electrocatalytic Performance in Overall Water Splitting with Rational Design of Hierarchical Co₃O₄@NiFe Layered Double Hydroxide Coreâ€Shell Nanostructure. ChemElectroChem, 2018, 5, 1357-1363.	1.7	34
113	First-Principles Study of Methanol Oxidation into Methyl Formate on Rutile TiO₂(110). Journal of Physical Chemistry C, 2014, 118, 19859-19868.	1.5	33
114	Defects, Adsorbates, and Photoactivity of Rutile TiO₂ (110): Insight by First-Principles Calculations. Journal of Physical Chemistry Letters, 2018, 9, 5281-5287.	2.1	33
115	Structural resolution of inorganic nanotubes with complex stoichiometry. Nature Communications, 2018, 9, 2033.	5.8	33
116	How Hole Injection Accelerates Both Ion Migration and Nonradiative Recombination in Metal Halide Perovskites. Journal of the American Chemical Society, 2022, 144, 6604-6612.	6.6	31
117	Reply to â€œComment on `Structure and dynamics of liquid water on rutile TiO2(110)'â€‰â€• Physical Review B, 2012, 85, .	1.1	30
118	Wurtzite-type CuInSe2 for high-performance solar cell absorber: ab initio exploration of the new phase structure. Journal of Materials Chemistry, 2012, 22, 21662.	6.7	30
119	Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. Journal of Applied Physics, 2014, 115, .	1.1	30
120	A first-principles study of lithium-decorated hybrid boron nitride and graphene domains for hydrogen storage. Journal of Chemical Physics, 2014, 141, 084711.	1.2	29
121	Ultrahigh capacitive performance of three-dimensional electrode nanomaterials based on Î±-MnO2 nanocrystallines induced by doping Au through Ã…-scale channels. Nano Energy, 2016, 21, 39-50.	8.2	29
122	The role of the defect on the adsorption and dissociation of water on graphitic carbon nitride. Applied Surface Science, 2015, 358, 363-369.	3.1	28
123	Structure and Oxygen Evolution Activity of Î²-NiOOH: Where Are the Protons?. ACS Catalysis, 2022, 12, 295-304.	5.5	28
124	Novel monolayer pyrite FeS2 with atomic-thickness for magnetic devices. Computational Materials Science, 2015, 101, 255-259.	1.4	27
125	Efficient design principle for interfacial charge separation in hydrogen-intercalated nonstoichiometric oxides. Nano Energy, 2018, 53, 887-897.	8.2	27
126	New insights into interfacial photocharge transfer in TiO₂/C₃N₄ heterostructures: effects of facets and defects. New Journal of Chemistry, 2019, 43, 4511-4517.	1.4	27

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127	Robust vanadium pentoxide electrodes for sodium and calcium ion batteries: thermodynamic and diffusion mechanical insights. Journal of Materials Chemistry A, 2016, 4, 12516-12525.	5.2	26
128	Increasing the band gap of FeS2 by alloying with Zn and applying biaxial strain: A first-principles study. Journal of Alloys and Compounds, 2015, 629, 43-48.	2.8	25
129	The microstructure, stability, and elastic properties of 14H long-period stacking-ordered phase in Mgâ€“Znâ€“Y alloys: a first-principles study. Journal of Materials Science, 2014, 49, 737-748.	1.7	24
130	Tunable band gap and magnetism of the two-dimensional nickel hydroxide. RSC Advances, 2015, 5, 77154-77158.	1.7	24
131	Tuning the electronic properties of half- and full-hydrogenated germanene by chlorination and hydroxylation: A first-principles study. Computational Materials Science, 2014, 92, 244-252.	1.4	23
132	Porous CoP nanosheet arrays grown on nickel foam as an excellent and stable catalyst for hydrogen evolution reaction. International Journal of Hydrogen Energy, 2017, 42, 26995-27003.	3.8	23
133	Water Film Adsorbed on the Î±-Al₂O₃(0001) Surface: Structural Properties and Dynamical Behaviors from First-Principles Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 5398-5409.	1.5	22
134	The predominant role of Zn6Y9 cluster in the long period stacking order structures of Mgâ€“Znâ€“Y alloys: a first-principles study. Journal of Materials Science, 2013, 48, 1407-1412.	1.7	20
135	Two-dimensional square-pyramidal VO₂ with tunable electronic properties. Journal of Materials Chemistry C, 2015, 3, 3189-3197.	2.7	20
136	The unique carrier mobility of Janus MoSSe/GaN heterostructures. Frontiers of Physics, 2021, 16, 1.	2.4	18
137	Atomic structure and electronic properties of folded graphene nanoribbons: A first-principles study. Journal of Applied Physics, 2013, 113, .	1.1	17
138	Cu₂ZnSnS₄ Nanocrystals as Highly Active and Stable Electrocatalysts for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2016, 120, 24265-24270.	1.5	17
139	Electric field and strain tunable electronic structures in monolayer Black Phosphorus. Computational Materials Science, 2016, 112, 297-303.	1.4	17
140	Solid wetting-layers in inorganic nano-reactors: the water in imogolite nanotube case. Nanoscale Advances, 2020, 2, 1869-1877.	2.2	17
141	Theoretical Study on the Composition Location of the Best Glass Formers in Cuâ€“Zr Amorphous Alloys. Journal of Physical Chemistry A, 2015, 119, 806-814.	1.1	16
142	Subnano Ruthenium Species Anchored on Tin Dioxide Surface for Efficient Alkaline Hydrogen Evolution Reaction. Cell Reports Physical Science, 2020, 1, 100026.	2.8	16
143	Inherent Simple Cubic Lattice Being Responsible for Ultrafast Solid-Phase Change of Ge₂Sb₂Te₅. Journal of Physical Chemistry Letters, 2017, 8, 2560-2564.	2.1	15
144	Direct observation of multiple rotational stacking faults coexisting in freestanding bilayer MoS2. Scientific Reports, 2017, 7, 8323.	1.6	15

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145	Effect of water on gas explosions: combined ReaxFF and ab initio MD calculations. RSC Advances, 2014, 4, 35048.	1.7	14
146	A low-surface energy carbon allotrope: the case for bcc-C₆. Physical Chemistry Chemical Physics, 2015, 17, 14083-14087.	1.3	13
147	Versatile electronic properties and exotic edge states of single-layer tetragonal silicon carbides. Physical Chemistry Chemical Physics, 2015, 17, 11211-11216.	1.3	13
148	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO₃ from First Principles. ACS Catalysis, 2019, 9, 10528-10535.	5.5	13
149	Activity and selectivity of CO₂ photoreduction on catalytic materials. Dalton Transactions, 2020, 49, 12918-12928.	1.6	13
150	Electrocatalysis enhancement of iron-based catalysts induced by synergy of methanol and oxygen-containing groups. Nano Energy, 2016, 21, 265-275.	8.2	12
151	Periodic continuum solvation model integrated with first-principles calculations for solid surfaces. Progress in Natural Science: Materials International, 2017, 27, 283-288.	1.8	12
152	Water-Hydrogen-Polaron Coupling at Anatase TiO2(101) Surfaces: A Hybrid Density Functional Theory Study. Journal of Physical Chemistry Letters, 2020, 11, 4317-4325.	2.1	12
153	Two-dimensional Ni(OH) ₂ -XS ₂ (X = Mo and W) heterostructures. 2D Materials, 2015, 2, 034014.	2.0	11
154	A strain or electric field induced direct bandgap in ultrathin silicon film and its application in photovoltaics or photocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 7156-7162.	1.3	11
155	The role of permanent and induced electrostatic dipole moments for Schottky barriers in Janus MXY/graphene heterostructures: a first-principles study. Dalton Transactions, 0, , .	1.6	11
156	Electronic and magnetism properties of two-dimensional stacked nickel hydroxides and nitrides. Scientific Reports, 2015, 5, 11656.	1.6	10
157	Effect of water on the effective Goldschmidt tolerance factor and photoelectric conversion efficiency of organicâ€“inorganic perovskite: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 14955-14960.	1.3	10
158	Theoretical Progress on the Relationship between the Structures and Properties of Perovskite Solar Cells. Advanced Theory and Simulations, 2020, 3, 2000022.	1.3	10
159	Bipolar doping of double-layer graphene vertical heterostructures with hydrogenated boron nitride. Physical Chemistry Chemical Physics, 2015, 17, 11692-11699.	1.3	9
160	Photoexcitation of bulk polarons in rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 103, .	1.1	9
161	The effects of subsurface Ov and Tiint of anatase (1â€0â€1) surface on CO2 conversion: A first-principles study. Computational Materials Science, 2018, 155, 424-430.	1.4	8
162	Spaceâ€Confined Creation of Nanoframes In Situ on Reduced Graphene Oxide. Small, 2015, 11, 1512-1518.	5.2	7

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163	Structure and reactivity of highly reduced titanium oxide surface layers on TiO2: A first-principles study. Journal of Chemical Physics, 2019, 151, 184701.	1.2	7
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