Li-Min Liu

List of Publications by Year in Descending Order

176 papers	12,259 citations	59 h-index	107 g-index
181 ext. papers	14,456 ext. citations	9.6 avg, IF	6.62 L-index

#	Paper	IF	Citations
176	Nonadiabatic Dynamics of Polaron Hopping and Coupling with Water on Reduced TiO.. *Journal of Physical Chemistry Letters*, **2022**, 857-863	6.4	1
175	The Role of Thermal Fluctuations and Vibrational Entropy: A Theoretical Insight into the □to-□ Transition of FAPbI.. *Journal of Physical Chemistry Letters*, **2022**, 3089-3095	6.4	0
174	How Hole Injection Accelerates Both Ion Migration and Nonradiative Recombination in Metal Halide Perovskites.. *Journal of the American Chemical Society*, **2022**,	16.4	14
173	Structure and Oxygen Evolution Activity of □NiOOH: Where Are the Protons?. *ACS Catalysis*, **2022**, 12, 295-304	13.1	2
172	Valence oscillation and dynamic active sites in monolayer NiCo hydroxides for water oxidation. *Nature Catalysis*, **2021**, 4, 1050-1058	36.5	46
171	Facet-Regulating Local Coordination of Dual-Atom Cocatalyzed TiO2 for Photocatalytic Water Splitting. *ACS Catalysis*, **2021**, 11, 14669-14676	13.1	4
170	Photoexcitation of bulk polarons in rutile TiO2. *Physical Review B*, **2021**, 103,	3.3	4
169	Amorphous Domains in Black Titanium Dioxide. *Advanced Materials*, **2021**, 33, e2100407	24	14
168	The unique carrier mobility of Janus MoSSe/GaN heterostructures. *Frontiers of Physics*, **2021**, 16, 1	3.7	5
167	New Insight of Pyrrole-Like Nitrogen for Boosting Hydrogen Evolution Activity and Stability of Pt Single Atoms. *Small*, **2021**, 17, e2004453	11	15
166	Water-Hydrogen-Polaron Coupling at Anatase TiO(101) Surfaces: A Hybrid Density Functional Theory Study. *Journal of Physical Chemistry Letters*, **2020**, 11, 4317-4325	6.4	9
165	Self-Induced Strain in 2D Chalcogenide Nanocrystals with Enhanced Photoelectrochemical Responsivity. *Chemistry of Materials*, **2020**, 32, 2774-2781	9.6	6
164	Solid wetting-layers in inorganic nano-reactors: the water in imogolite nanotube case. *Nanoscale Advances*, **2020**, 2, 1869-1877	5.1	11
163	Theoretical Progress on the Relationship between the Structures and Properties of Perovskite Solar Cells. *Advanced Theory and Simulations*, **2020**, 3, 2000022	3.5	4
162	Synergy between Ion Migration and Charge Carrier Recombination in Metal-Halide Perovskites. *Journal of the American Chemical Society*, **2020**, 142, 3060-3068	16.4	55
161	Subnano Ruthenium Species Anchored on Tin Dioxide Surface for Efficient Alkaline Hydrogen Evolution Reaction. *Cell Reports Physical Science*, **2020**, 1, 100026	6.1	10
160	Site dependent reactivity of Pt single atoms on anatase TiO(101) in an aqueous environment. *Physical Chemistry Chemical Physics*, **2020**, 22, 10455-10461	3.6	4

159	Engineering the Low Coordinated Pt Single Atom to Achieve the Superior Electrocatalytic Performance toward Oxygen Reduction. *Small*, **2020**, 16, e2003096	11	36
158	The oxygen vacancy in Li-ion battery cathode materials. *Nanoscale Horizons*, **2020**, 5, 1453-1466	10.8	24
157	Activity and selectivity of CO photoreduction on catalytic materials. *Dalton Transactions*, **2020**, 49, 12918-12928	4.3	7
156	-60 °C solution synthesis of atomically dispersed cobalt electrocatalyst with superior performance. *Nature Communications*, **2019**, 10, 606	17.4	87
155	Injection of oxygen vacancies in the bulk lattice of layered cathodes. *Nature Nanotechnology*, **2019**, 14, 602-608	28.7	180
154	The Influence of Dipole Moments Induced by Organic Molecules and Domain Structures on the Properties of CH3NH3PbI3 Perovskite. *Advanced Theory and Simulations*, **2019**, 2, 1900041	3.5	4
153	Rational molecular passivation for high-performance perovskite light-emitting diodes. *Nature Photonics*, **2019**, 13, 418-424	33.9	638
152	New insights into interfacial photocharge transfer in TiO2/C3N4 heterostructures: effects of facets and defects. *New Journal of Chemistry*, **2019**, 43, 4511-4517	3.6	21
151	Defect Modulation of Z-Scheme TiO2/Cu2O Photocatalysts for Durable Water Splitting. *ACS Catalysis*, **2019**, 9, 8346-8354	13.1	86
150	Understanding the Influence of Cation Doping on the Surface Chemistry of NaTaO3from First Principles. *ACS Catalysis*, **2019**, 9, 10528-10535	13.1	6
149	Atomic layer deposited Pt-Ru dual-metal dimers and identifying their active sites for hydrogen evolution reaction. *Nature Communications*, **2019**, 10, 4936	17.4	186
148	Structure and reactivity of highly reduced titanium oxide surface layers on TiO: A first-principles study. *Journal of Chemical Physics*, **2019**, 151, 184701	3.9	4
147	Effect of Single-Atom Cocatalysts on the Activity of Faceted TiO Photocatalysts. *Langmuir*, **2019**, 35, 391-397	4	27
146	Rational Design of Ultrasmall Au Nanoparticles on Fe via Galvanic Replacement Under 60 °C for Efficient Methanol Oxidation Reaction Catalyst. *ACS Applied Energy Materials*, **2019**, 2, 468-476	6.1	1
145	Tailor-made metal-nitrogen-carbon bifunctional electrocatalysts for rechargeable Zn-air batteries via controllable MOF units. *Energy Storage Materials*, **2019**, 17, 46-61	19.4	42
144	Improved Electrocatalytic Performance in Overall Water Splitting with Rational Design of Hierarchical Co3O4@NiFe Layered Double Hydroxide Core-Shell Nanostructure. *ChemElectroChem*, **2018**, 5, 1357-1363	4.3	27
143	Tuning defects in oxides at room temperature by lithium reduction. *Nature Communications*, **2018**, 9, 1302	17.4	225
142	Well-Dispersed Ruthenium in Mesoporous Crystal TiO as an Advanced Electrocatalyst for Hydrogen Evolution Reaction. *Journal of the American Chemical Society*, **2018**, 140, 5719-5727	16.4	152

141	A highly stable bifunctional catalyst based on 3D Co(OH)2@NCNTs@NF towards overall water-splitting. *Nano Energy*, **2018**, 47, 96-104	17.1	94
140	Excess electrons in reduced rutile and anatase TiO2. *Surface Science Reports*, **2018**, 73, 58-82	12.9	75
139	Ice Melting to Release Reactants in Solution Syntheses. *Angewandte Chemie - International Edition*, **2018**, 57, 3354-3359	16.4	24
138	Tunable dipole and carrier mobility for a few layer Janus MoSSe structure. *Journal of Materials Chemistry C*, **2018**, 6, 1693-1700	7.1	106
137	Improved Electrocatalytic Performance in Overall Water Splitting with Rational Design of Hierarchical Co3O4@NiFe Layered Double Hydroxide Core–Shell Nanostructure. *ChemElectroChem*, **2018**, 5, 1339-1339	4.3	
136	Optical properties and applications for MoS2-Sb2Te3-MoS2heterostructure materials. *Photonics Research*, **2018**, 6, 220	6	111
135	Janus MoSSe Nanotubes: Tunable Band Gap and Excellent Optical Properties for Surface Photocatalysis. *Advanced Theory and Simulations*, **2018**, 1, 1800082	3.5	23
134	Long Carrier Lifetimes in PbI2-Rich Perovskites Rationalized by Ab Initio Nonadiabatic Molecular Dynamics. *ACS Energy Letters*, **2018**, 3, 1868-1874	20.1	41
133	Multi-electric field modulation for photocatalytic oxygen evolution: Enhanced charge separation by coupling oxygen vacancies with faceted heterostructures. *Nano Energy*, **2018**, 51, 764-773	17.1	68
132	Self-hydrogenated shell promoting photocatalytic H evolution on anatase TiO. *Nature Communications*, **2018**, 9, 2752	17.4	111
131	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	17.1	111
130	The effects of subsurface Ov and Tiint of anatase (1 0 1) surface on CO2 conversion: A first-principles study. *Computational Materials Science*, **2018**, 155, 424-430	3.2	6
129	Efficient design principle for interfacial charge separation in hydrogen-intercalated nonstoichiometric oxides. *Nano Energy*, **2018**, 53, 887-897	17.1	24
128	Defects, Adsorbates, and Photoactivity of Rutile TiO (110): Insight by First-Principles Calculations. *Journal of Physical Chemistry Letters*, **2018**, 9, 5281-5287	6.4	25
127	Structural resolution of inorganic nanotubes with complex stoichiometry. *Nature Communications*, **2018**, 9, 2033	17.4	22
126	Electronic structure and photoabsorption of Ti ions in reduced anatase and rutile TiO. *Physical Chemistry Chemical Physics*, **2018**, 20, 17658-17665	3.6	27
125	First-Principles Study of Novel Two-Dimensional (CHNH)PbX Perovskites for Solar Cell Absorbers. *Journal of Physical Chemistry Letters*, **2017**, 8, 876-883	6.4	46
124	Periodic continuum solvation model integrated with first-principles calculations for solid surfaces. *Progress in Natural Science: Materials International*, **2017**, 27, 283-288	3.6	10

123	Effect of water on the effective Goldschmidt tolerance factor and photoelectric conversion efficiency of organic-inorganic perovskite: insights from first-principles calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 14955-14960	3.6	6
122	Inherent Simple Cubic Lattice Being Responsible for Ultrafast Solid-Phase Change of GeSbTe. *Journal of Physical Chemistry Letters*, **2017**, 8, 2560-2564	6.4	10
121	Boosting photoelectrochemical activities of heterostructured photoanodes through interfacial modulation of oxygen vacancies. *Nano Energy*, **2017**, 35, 290-298	17.1	43
120	Formation of New Phases to Improve the Visible-Light Photocatalytic Activity of Tio2 (B) Via Introducing Alien Elements. *Journal of Physical Chemistry C*, **2017**, 121, 52-59	3.8	1
119	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	6.7	20
118	Direct observation of multiple rotational stacking faults coexisting in freestanding bilayer MoS. *Scientific Reports*, **2017**, 7, 8323	4.9	11
117	Enhanced optical absorption via cation doping hybrid lead iodine perovskites. *Scientific Reports*, **2017**, 7, 7843	4.9	39
116	Role of Methylammonium Orientation in Ion Diffusion and Current□Voltage Hysteresis in the CH3NH3PbI3 Perovskite. *ACS Energy Letters*, **2017**, 2, 1997-2004	20.1	55
115	Iced photochemical reduction to synthesize atomically dispersed metals by suppressing nanocrystal growth. *Nature Communications*, **2017**, 8, 1490	17.4	219
114	Surface evolution of a Pt□Pd□Au electrocatalyst for stable oxygen reduction. *Nature Energy*, **2017**, 2,	62.3	233
113	Tuning band gaps and optical absorption of BiOCl through doping and strain: insight form DFT calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 20968-20973	3.6	25
112	Cu2ZnSnS4 Nanocrystals as Highly Active and Stable Electrocatalysts for the Oxygen Reduction Reaction. *Journal of Physical Chemistry C*, **2016**, 120, 24265-24270	3.8	13
111	Unusual Li-Ion Transfer Mechanism in Liquid Electrolytes: A First-Principles Study. *Journal of Physical Chemistry Letters*, **2016**, 7, 4795-4801	6.4	27
110	Thiolate-Mediated Photoinduced Synthesis of Ultrafine Ag S Quantum Dots from Silver Nanoparticles. *Angewandte Chemie - International Edition*, **2016**, 55, 14952-14957	16.4	33
109	A sulfur host based on titanium monoxide@carbon hollow spheres for advanced lithium-sulfur batteries. *Nature Communications*, **2016**, 7, 13065	17.4	511
108	Structures and Electronic Properties of Different CH3NH3PbI3/TiO2 Interface: A First-Principles Study. *Scientific Reports*, **2016**, 6, 20131	4.9	60
107	Spatial separation of photo-generated electron-hole pairs in BiOBr/BiOI bilayer to facilitate water splitting. *Scientific Reports*, **2016**, 6, 32764	4.9	44
106	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	13	39

105	Multifunctional Nitrogen-Doped Loofah Sponge Carbon Blocking Layer for High-Performance Rechargeable Lithium Batteries. *ACS Applied Materials & Interfaces*, **2016**, 8, 15991-6001	9.5	52
104	Ultrahigh capacitive performance of three-dimensional electrode nanomaterials based on MnO2 nanocrystallines induced by doping Au through scale channels. *Nano Energy*, **2016**, 21, 39-50	17.1	29
103	Phosphorene ribbons as anode materials with superhigh rate and large capacity for Li-ion batteries. *Journal of Power Sources*, **2016**, 302, 215-222	8.9	37
102	Electrocatalysis enhancement of iron-based catalysts induced by synergy of methanol and oxygen-containing groups. *Nano Energy*, **2016**, 21, 265-275	17.1	10
101	Potential Application of Metal Dichalcogenides Double-Layered Heterostructures as Anode Materials for Li-Ion Batteries. *Journal of Physical Chemistry C*, **2016**, 120, 4779-4788	3.8	59
100	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, 7156-62	3.6	11
99	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	6.7	68
98	Electric field and strain tunable electronic structures in monolayer Black Phosphorus. *Computational Materials Science*, **2016**, 112, 297-303	3.2	10
97	Robust vanadium pentoxide electrodes for sodium and calcium ion batteries: thermodynamic and diffusion mechanical insights. *Journal of Materials Chemistry A*, **2016**, 4, 12516-12525	13	22
96	New Insights into Defect-Mediated Heterostructures for Photoelectrochemical Water Splitting. *Advanced Energy Materials*, **2016**, 6, 1502268	21.8	75
95	Enhanced Thermoelectric Properties of Cu2SnSe3 by (Ag,In)-Co-Doping. *Advanced Functional Materials*, **2016**, 26, 6025-6032	15.6	59
94	Platinum single-atom and cluster catalysis of the hydrogen evolution reaction. *Nature Communications*, **2016**, 7, 13638	17.4	1085
93	The Effect of Excess Electron and hole on CO2 Adsorption and Activation on Rutile (110) surface. *Scientific Reports*, **2016**, 6, 23298	4.9	29
92	Water at Interfaces. *Chemical Reviews*, **2016**, 116, 7698-726	68.1	388
91	Ultra-small B2O3 nanocrystals grown in situ on highly porous carbon microtubes for lithium iodine and lithium sulfur batteries. *Journal of Materials Chemistry A*, **2016**, 4, 8541-8547	13	54
90	Water Film Adsorbed on the Al2O3(0001) Surface: Structural Properties and Dynamical Behaviors from First-Principles Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 5398-5409	4.8	20
89	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	6.7	58
88	An electron injection promoted highly efficient electrocatalyst of FeNi3@GR@Fe-NiOOH for oxygen evolution and rechargeable metal air batteries. *Journal of Materials Chemistry A*, **2016**, 4, 7762-7771	13	55

87	Phenylalkylamine Passivation of Organolead Halide Perovskites Enabling High-Efficiency and Air-Stable Photovoltaic Cells. *Advanced Materials*, **2016**, 28, 9986-9992	24	425
86	Substitution Boosts Charge Separation for High Solar-Driven Photocatalytic Performance. *ACS Applied Materials & Interfaces*, **2016**, 8, 26783-26793	9.5	30
85	Space-confined creation of nanoframes in situ on reduced graphene oxide. *Small*, **2015**, 11, 1512-8	11	6
84	Two-dimensional square-pyramidal VO2 with tunable electronic properties. *Journal of Materials Chemistry C*, **2015**, 3, 3189-3197	7.1	16
83	An ab initio study of TiS3: a promising electrode material for rechargeable Li and Na ion batteries. *RSC Advances*, **2015**, 5, 21455-21463	3.7	49
82	Porous structure design of carbon xerogels for advanced supercapacitor. *Applied Energy*, **2015**, 153, 32-40	6.7	29
81	Novel monolayer pyrite FeS2 with atomic-thickness for magnetic devices. *Computational Materials Science*, **2015**, 101, 255-259	3.2	14
80	Effect of Surface Structure on the Photoreactivity of TiO2. *Journal of Physical Chemistry C*, **2015**, 119, 6121-6127	3.8	41
79	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	3.8	97
78	Dynamic Responses and Initial Decomposition under Shock Loading: A DFTB Calculation Combined with MSST Method for β-HMX with Molecular Vacancy. *Journal of Physical Chemistry B*, **2015**, 119, 10673-81	3.4	35
77	Coverage Dependence of Methanol Dissociation on TiO(110). *Journal of Physical Chemistry Letters*, **2015**, 6, 3327-3334	6.4	51
76	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	6.4	147
75	Effect of surface composition on electronic properties of methylammonium lead iodide perovskite. *Journal of Materiomics*, **2015**, 1, 213-220	6.7	42
74	The role of the defect on the adsorption and dissociation of water on graphitic carbon nitride. *Applied Surface Science*, **2015**, 358, 363-369	6.7	20
73	A porous nitrogen and phosphorous dual doped graphene blocking layer for high performance Li-S batteries. *Journal of Materials Chemistry A*, **2015**, 3, 16670-16678	13	219
72	Localized Excitation of Ti(3+) Ions in the Photoabsorption and Photocatalytic Activity of Reduced Rutile TiO2. *Journal of the American Chemical Society*, **2015**, 137, 9146-52	16.4	139
71	Electronic and magnetism properties of two-dimensional stacked nickel hydroxides and nitrides. *Scientific Reports*, **2015**, 5, 11656	4.9	8
70	Pristine and defect-containing phosphorene as promising anode materials for rechargeable Li batteries. *Journal of Materials Chemistry A*, **2015**, 3, 11246-11252	13	112

69	A low-surface energy carbon allotrope: the case for bcc-C6. *Physical Chemistry Chemical Physics*, **2015**, 17, 14083-7	3.6	9
68	Versatile electronic properties and exotic edge states of single-layer tetragonal silicon carbides. *Physical Chemistry Chemical Physics*, **2015**, 17, 11211-6	3.6	12
67	Two-dimensional hexagonal V2O nanosheet and nanoribbons. *Applied Physics Express*, **2015**, 8, 035201	2.4	
66	Porous BN for hydrogen generation and storage. *Journal of Materials Chemistry A*, **2015**, 3, 9632-9637	13	65
65	Tunable band gap and magnetism of the two-dimensional nickel hydroxide. *RSC Advances*, **2015**, 5, 77154-77158	3.7	38
64	First-Principles Study of Phosphorene and Graphene Heterostructure as Anode Materials for Rechargeable Li Batteries. *Journal of Physical Chemistry Letters*, **2015**, 6, 5002-8	6.4	215
63	Two-dimensional Ni(OH) 2 -XS 2 (X = Mo and W) heterostructures. *2D Materials*, **2015**, 2, 034014	5.9	9
62	Hierarchical NiCo2 O4 nanosheets grown on Ni nanofoam as high-performance electrodes for supercapacitors. *Small*, **2015**, 11, 804-8	11	211
61	Visible-light induced photocatalytic activity of electrospun-TiO2 in arsenic(III) oxidation. *ACS Applied Materials & Interfaces*, **2015**, 7, 511-8	9.5	39
60	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
59	Formation of Bi2WO6 Bipyramids with Vacancy Pairs for Enhanced Solar-Driven Photoactivity. *Advanced Functional Materials*, **2015**, 25, 3726-3734	15.6	117
58	Hierarchical three-dimensional NiCo2O4 nanoneedle arrays supported on Ni foam for high-performance supercapacitors. *RSC Advances*, **2015**, 5, 25304-25311	3.7	51
57	High carrier mobility of few-layer PbX (X = S, Se, Te). *Journal of Materials Chemistry C*, **2015**, 3, 6284-6290	7.1	29
56	Bipolar doping of double-layer graphene vertical heterostructures with hydrogenated boron nitride. *Physical Chemistry Chemical Physics*, **2015**, 17, 11692-9	3.6	8
55	Ultrathin NiCo2O4 nanosheets 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	13	68
54	Structures, stabilities, and electronic properties of defects in monolayer black phosphorus. *Scientific Reports*, **2015**, 5, 10848	4.9	72
53	CO2 Capture and Conversion on Rutile TiO2(110) in the Water Environment: Insight by First-Principles Calculations. *Journal of Physical Chemistry Letters*, **2015**, 6, 2538-45	6.4	49
52	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	5.7	18

51	Theoretical study on the composition location of the best glass formers in Cu-Zr amorphous alloys. *Journal of Physical Chemistry A*, **2015**, 119, 806-14	2.8	14
50	The stability and electronic properties of novel three-dimensional graphene-MoS2 hybrid structure. *Scientific Reports*, **2014**, 4, 7007	4.9	37
49	The microstructure, stability, and elastic properties of 14H long-period stacking-ordered phase in Mg□Zn□ alloys: a first-principles study. *Journal of Materials Science*, **2014**, 49, 737-748	4.3	19
48	Modulating the atomic and electronic structures through alloying and heterostructure of single-layer MoS2. *Journal of Materials Chemistry A*, **2014**, 2, 2101-2109	13	69
47	The effect of water on the structural, electronic and photocatalytic properties of graphitic carbon nitride. *Physical Chemistry Chemical Physics*, **2014**, 16, 3299-304	3.6	85
46	From melamine□resorcinol□formaldehyde to nitrogen-doped carbon xerogels with micro- and meso-pores for lithium batteries. *Journal of Materials Chemistry A*, **2014**, 2, 14429-14438	13	58
45	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. *Physical Chemistry Chemical Physics*, **2014**, 16, 25854-61	3.6	90
44	New manifold two-dimensional single-layer structures of zinc-blende compounds. *Journal of Materials Chemistry A*, **2014**, 2, 17971-17978	13	92
43	Effect of water on gas explosions: combined ReaxFF and ab initio MD calculations. *RSC Advances*, **2014**, 4, 35048	3.7	11
42	Si doping at GaN inversion domain boundaries: an interfacial polar field for electron and hole separation. *Journal of Materials Chemistry A*, **2014**, 2, 9744	13	4
41	Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion. *Journal of Materials Chemistry A*, **2014**, 2, 15389-15395	13	71
40	Single-layer Group-IVB nitride halides as promising photocatalysts. *Journal of Materials Chemistry A*, **2014**, 2, 6755	13	69
39	Two dimensional Dirac carbon allotropes from graphene. *Nanoscale*, **2014**, 6, 1113-8	7.7	147
38	First-Principles Study of Methanol Oxidation into Methyl Formate on Rutile TiO2(110). *Journal of Physical Chemistry C*, **2014**, 118, 19859-19868	3.8	27
37	A novel three dimensional semimetallic MoS2. *Journal of Applied Physics*, **2014**, 115, 204302	2.5	4
36	First-Principles Study of Lead Iodide Perovskite Tetragonal and Orthorhombic Phases for Photovoltaics. *Journal of Physical Chemistry C*, **2014**, 118, 19565-19571	3.8	196
35	Doping high-surface-area mesoporous TiO2 microspheres with carbonate for visible light hydrogen production. *Energy and Environmental Science*, **2014**, 7, 2592	35.4	232
34	Band gap engineering of FeS2 under biaxial strain: a first principles study. *Physical Chemistry Chemical Physics*, **2014**, 16, 24466-72	3.6	31

33	The intrinsic mechanism of methane oxidation under explosion condition: A combined ReaxFF and DFT study. *Fuel*, **2014**, 124, 85-90	7.1	65
32	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	3.2	17
31	Oxygen-doped boron nitride nanosheets with excellent performance in hydrogen storage. *Nano Energy*, **2014**, 6, 219-224	17.1	170
30	Diverse and tunable electronic structures of single-layer metal phosphorus trichalcogenides for photocatalytic water splitting. *Journal of Chemical Physics*, **2014**, 140, 054707	3.9	76
29	Adaptive cluster expansion approach for predicting the structure evolution of graphene oxide. *Journal of Chemical Physics*, **2014**, 141, 224703	3.9	2
28	Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. *Journal of Applied Physics*, **2014**, 115, 093504	2.5	23
27	A first-principles study of lithium-decorated hybrid boron nitride and graphene domains for hydrogen storage. *Journal of Chemical Physics*, **2014**, 141, 084711	3.9	22
26	Atomic structure and electronic properties of folded graphene nanoribbons: A first-principles study. *Journal of Applied Physics*, **2013**, 113, 173506	2.5	13
25	Tunable electronic and magnetic properties of WS2 nanoribbons. *Journal of Applied Physics*, **2013**, 114, 093710	2.5	37
24	Ab initio molecular dynamics simulation on the formation process of He@C□synthesized by explosion. *Journal of Molecular Modeling*, **2013**, 19, 1705-10	2	2
23	Band-Gap States of TiO2(110): Major Contribution from Surface Defects. *Journal of Physical Chemistry Letters*, **2013**, 4, 3839-3844	6.4	62
22	Dimension-dependent phase transition and magnetic properties of VS2. *Journal of Materials Chemistry A*, **2013**, 1, 10821	13	154
21	The predominant role of Zn6Y9 cluster in the long period stacking order structures of Mg□nY alloys: a first-principles study. *Journal of Materials Science*, **2013**, 48, 1407-1412	4.3	17
20	R-graphyne: a new two-dimensional carbon allotrope with versatile Dirac-like point in nanoribbons. *Journal of Materials Chemistry A*, **2013**, 1, 5341	13	90
19	□MnO2 as a cathode material for lithium ion batteries from first principles calculations. *Physical Chemistry Chemical Physics*, **2013**, 15, 9075-83	3.6	62
18	Why Clorine Is an Inefficient n-Type Dopant in CuInSe2?. *Japanese Journal of Applied Physics*, **2013**, 52, 100208	1.4	
17	Enhanced thermal decomposition of nitromethane on functionalized graphene sheets: ab initio molecular dynamics simulations. *Journal of the American Chemical Society*, **2012**, 134, 19011-6	16.4	72
16	Two-Dimensional Superlattice: Modulation of Band Gaps in Graphene-Based Monolayer Carbon Superlattices. *Journal of Physical Chemistry Letters*, **2012**, 3, 3373-3378	6.4	52

15	Wurtzite-type CuInSe2 for high-performance solar cell absorber: ab initio exploration of the new phase structure. *Journal of Materials Chemistry*, **2012**, 22, 21662		26
14	Thermal transport in graphyne nanoribbons. *Physical Review B*, **2012**, 85,	3.3	95
13	Reply to Comment on 'Structure and dynamics of liquid water on rutile TiO2(110)' *Physical Review B*, **2012**, 85,	3.3	28
12	Growth and organization of an organic molecular monolayer on TiO2: catechol on anatase (101). *Journal of the American Chemical Society*, **2011**, 133, 7816-23	16.4	93
11	Melting the ice: on the relation between melting temperature and size for nanoscale ice crystals. *ACS Nano*, **2011**, 5, 4562-9	16.7	59
10	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2011**, 13, 13162-6	3.6	41
9	Surface energy and surface proton order of the ice Ih basal and prism surfaces. *Journal of Physics Condensed Matter*, **2010**, 22, 074209	1.8	35
8	Structure and dynamics of liquid water on rutile TiO2(110). *Physical Review B*, **2010**, 82,	3.3	162
7	Titania-water interactions: a review of theoretical studies. *Journal of Materials Chemistry*, **2010**, 20, 10319		228
6	Interfacial water: a first principles molecular dynamics study of a nanoscale water film on salt. *Journal of Chemical Physics*, **2009**, 130, 234702	3.9	44
5	The interaction between adsorbed OH and O2 on TiO2 surfaces. *Progress in Surface Science*, **2009**, 84, 155-176	6.6	111
4	Surface energy and surface proton order of ice Ih. *Physical Review Letters*, **2008**, 101, 155703	7.4	65
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