Chuying Ouyang

List of Publications by Citations

187 papers	6,859 citations	44 h-index	77 g-index
191 ext. papers	7,962 ext. citations	4.9 avg, IF	6.15 L-index

#	Paper	IF	Citations
187	Multi-scale computation methods: Their applications in lithium-ion battery research and development. *Chinese Physics B*, **2016**, 25, 018212	1.2	346
186	Trace doping of multiple elements enables stable battery cycling of LiCoO2 at 4.6 V. *Nature Energy*, **2019**, 4, 594-603	62.3	299
185	Ab initio studies of structural and electronic properties of Li4Ti5O12 spinel. *Electrochemistry Communications*, **2007**, 9, 1107-1112	5.1	239
184	Designing Air-Stable O3-Type Cathode Materials by Combined Structure Modulation for Na-Ion Batteries. *Journal of the American Chemical Society*, **2017**, 139, 8440-8443	16.4	219
183	Enhancement of electronic conductivity of LiFePO4 by Cr doping and its identification by first-principles calculations. *Physical Review B*, **2003**, 68,	3.3	219
182	Investigations on V2C and V2CX2 (X = F, OH) Monolayer as a Promising Anode Material for Li Ion Batteries from First-Principles Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 24274-24281	3.8	215
181	First-principles study of Li ion diffusion in LiFePO4. *Physical Review B*, **2004**, 69,	3.3	209
180	Synthesis and Lithium Storage Mechanism of Ultrafine MoO2 Nanorods. *Chemistry of Materials*, **2012**, 24, 457-463	9.6	201
179	Ab initio studies on atomic and electronic structures of black phosphorus. *Journal of Applied Physics* , **2010**, 107, 093718	2.5	200
178	Effect of cation substitution on the pseudocapacitive performance of spinel cobaltite MCo2O4 (M = Mn, Ni, Cu, and Co). *Journal of Materials Chemistry A*, **2018**, 6, 10674-10685	13	164
177	Jahn□eller distortion and electronic structure of LiMn2O4. *Journal of Alloys and Compounds*, **2009**, 474, 370-374	5.7	133
176	2D Electrides as Promising Anode Materials for Na-Ion Batteries from First-Principles Study. *ACS Applied Materials & Interfaces*, **2015**, 7, 24016-22	9.5	126
175	Nitrogen- and Phosphorus-Doped Biocarbon with Enhanced Electrocatalytic Activity for Oxygen Reduction. *ACS Catalysis*, **2015**, 5, 920-927	13.1	124
174	Effect of Co Content on Rate Performance of LiMn[sub 0.5□]Co[sub 2x]Ni[sub 0.5□]O[sub 2] Cathode Materials for Lithium-Ion Batteries. *Journal of the Electrochemical Society*, **2004**, 151, A504	3.9	123
173	Electrical and Lithium Ion Dynamics in Three Main Components of Solid Electrolyte Interphase from Density Functional Theory Study. *Journal of Physical Chemistry C*, **2011**, 115, 7044-7049	3.8	117
172	First-principles study of the oxygen adsorption and dissociation on graphene and nitrogen doped graphene for Li-air batteries. *Journal of Applied Physics*, **2012**, 112, 104316	2.5	112
171	New insight into the effect of fluorine doping and oxygen vacancies on electrochemical performance of Co2MnO4 for flexible quasi-solid-state asymmetric supercapacitors. *Energy Storage Materials*, **2019**, 22, 384-396	19.4	105

170	First-principles investigation on redox properties of M-doped CeO2 (M=Mn,Pr,Sn,Zr). *Physical Review B*, **2010**, 82,	3.3	100
169	Improving the Electrochemical Activity of LiMnPO[sub 4] Via Mn-Site Substitution. *Journal of the Electrochemical Society*, **2010**, 157, A225	3.9	98
168	Investigations on Nb2C monolayer as promising anode material for Li or non-Li ion batteries from first-principles calculations. *RSC Advances*, **2016**, 6, 27467-27474	3.7	96
167	Ab initio studies on Li4+xTi5O12 compounds as anode materials for lithium-ion batteries. *ChemPhysChem*, **2008**, 9, 2104-8	3.2	95
166	Phosphorous-containing oxygen-deficient cobalt molybdate as an advanced electrode material for supercapacitors. *Energy Storage Materials*, **2019**, 19, 186-196	19.4	90
165	Theoretical study of cation doping effect on the electronic conductivity of Li4Ti5O12. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 1835-1841	1.3	77
164	First principles study of Jahn□eller effects in LixMnPO4. *Solid State Communications*, **2010**, 150, 40-44	1.6	76
163	First-principles study of high-capacity hydrogen storage on graphene with Li atoms. *Journal of Physics and Chemistry of Solids*, **2012**, 73, 245-251	3.9	74
162	Tailoring Lithium Deposition via an SEI-Functionalized Membrane Derived from LiF Decorated Layered Carbon Structure. *Advanced Energy Materials*, **2019**, 9, 1802912	21.8	74
161	Strain tuned Li diffusion in LiCoO2 material for Li ion batteries: A first principles study. *Solid State Ionics*, **2014**, 263, 46-48	3.3	71
160	Strain-induced semimetal-metal transition in silicene. *Europhysics Letters*, **2012**, 99, 17010	1.6	70
159	Geometry and fast diffusion of AlCl4 cluster intercalated in graphite. *Electrochimica Acta*, **2016**, 195, 158-165	6.7	69
158	The effect of Cr doping on Li ion diffusion in LiFePO4from first principles investigations and Monte Carlo simulations. *Journal of Physics Condensed Matter*, **2004**, 16, 2265-2272	1.8	68
157	Effect of Mg-doping on the structural and electronic properties of LiCoO2: A first-principles investigation. *Journal of Power Sources*, **2007**, 171, 908-912	8.9	66
156	Siligraphene as a promising anode material for lithium-ion batteries predicted from first-principles calculations. *Nano Energy*, **2018**, 49, 67-76	17.1	65
155	Oxidation States of Mn Atoms at Clean and Al2O3-Covered LiMn2O4(001) Surfaces. *Journal of Physical Chemistry C*, **2010**, 114, 4756-4759	3.8	63
154	W6+ & Br□odoped Li4Ti5O12 anode with super rate performance for Li-ion batteries. *Journal of Materials Chemistry A*, **2015**, 3, 13706-13716	13	59
153	Li-decorated graphyne as high-capacity hydrogen storage media: First-principles plane wave calculations. *International Journal of Hydrogen Energy*, **2014**, 39, 17104-17111	6.7	56

152	Ce3+-doped Li4Ti5O12 with CeO2 surface modification by a sol-gel method for high-performance lithium-ion batteries. *Electrochimica Acta*, **2016**, 189, 147-157	6.7	55
151	Phosphorus-Mediated MoS Nanowires as a High-Performance Electrode Material for Quasi-Solid-State Sodium-Ion Intercalation Supercapacitors. *Small*, **2019**, 15, e1803984	11	54
150	Ab initio molecular-dynamics studies on Li x Mn 2 O 4 as cathode material for lithium secondary batteries. *Europhysics Letters*, **2004**, 67, 28-34	1.6	53
149	First-principles investigation of the structural, magnetic, and electronic properties of olivine LiFePO4. *Physical Review B*, **2005**, 71,	3.3	50
148	First-principles investigation of transition metal atom M (M = Cu, Ag, Au) adsorption on CeO2(110). *Physical Chemistry Chemical Physics*, **2012**, 14, 1923-33	3.6	47
147	The effect of cation doping on spinel LiMn2O4: a first-principles investigation. *Solid State Communications*, **2003**, 126, 531-534	1.6	47
146	Tunable electronic structures in BP/MoSSe van der Waals heterostructures by external electric field and strain. *Applied Surface Science*, **2019**, 497, 143809	6.7	45
145	First-principles study of lattice dynamics of LiFePO4. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 4096-4100	2.3	45
144	Hydrogen-induced interactions in vanadium from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	44
143	Lithium ion diffusion in Li4+xTi5O12: From ab initio studies. *Electrochimica Acta*, **2011**, 56, 6084-6088	6.7	44
142	Antisite defects and Mg doping in LiFePO4: a first-principles investigation. *Applied Physics A: Materials Science and Processing*, **2011**, 104, 529-537	2.6	43
141	First-principles investigation of the bonding, optical and lattice dynamical properties of CeO2. *Journal of Power Sources*, **2009**, 194, 830-834	8.9	43
140	Electronic states of metal (Cu, Ag, Au) atom on CeO2(111) surface: The role of local structural distortion. *Journal of Power Sources*, **2012**, 197, 28-37	8.9	41
139	First Principles Study on Na x Li 1−x FePO 4 As Cathode Material for Rechargeable Lithium Batteries. *Chinese Physics Letters*, **2006**, 23, 61-64	1.8	39
138	Small polaron migration in LixMn2O4: From first principles calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 2796-2799	2.3	37
137	Crystal structure and electrochemical characteristics of non-AB5 type La–Ni system alloys. *Journal of Power Sources*, **2007**, 164, 911-915	8.9	37
136	Germagraphene as a promising anode material for lithium-ion batteries predicted from first-principles calculations. *Nanoscale Horizons*, **2019**, 4, 457-463	10.8	36
135	First-principles study of α-Al2O3 (100) surface. *Physical Review B*, **2009**, 79,	3.3	34

134	Theoretical Prediction of Janus MoSSe as a Potential Anode Material for Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2018**, 122, 23899-23909	3.8	34
133	Bulk properties and transport mechanisms of a solid state antiperovskite Li-ion conductor Li3OCl: insights from first principles calculations. *Journal of Materials Chemistry A*, **2018**, 6, 1150-1160	13	33
132	Bandgap tuning in MoSSe bilayers: synergistic effects of dipole moment and interlayer distance. *Physical Chemistry Chemical Physics*, **2018**, 20, 20919-20926	3.6	32
131	Ab initio investigation of the surface properties of Cu(111) and Li diffusion in Cu thin film. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2005**, 337, 247-255	2.3	32
130	Mechanical properties of W□i alloys from first-principles calculations. *Fusion Engineering and Design*, **2016**, 106, 34-39	1.7	29
129	Coordination of lithium ion with ethylene carbonate electrolyte solvent: A computational study. *International Journal of Quantum Chemistry*, **2016**, 116, 97-102	2.1	29
128	Three-dimensional honeycomb carbon: Junction line distortion and novel emergent fermions. *Carbon*, **2019**, 141, 417-426	10.4	29
127	Insights into structural stability and Li superionic conductivity of Li10GeP2S12 from first-principles calculations. *Chemical Physics Letters*, **2014**, 591, 16-20	2.5	28
126	Structural, Electronic, and Li Migration Properties of RE-Doped (RE = Ce, La) LiCoO2 for Li-ion Batteries: A First-Principles Investigation. *Journal of Physical Chemistry C*, **2016**, 120, 18428-18434	3.8	28
125	Multiple Dirac Points and Hydrogenation-Induced Magnetism of Germanene Layer on Al (111) Surface. *Journal of Physical Chemistry Letters*, **2015**, 6, 4936-42	6.4	27
124	Physics of electron and lithium-ion transport in electrode materials for Li-ion batteries. *Chinese Physics B*, **2016**, 25, 018206	1.2	27
123	Charge transfer and formation of Ce3+ upon adsorption of metal atom M (M□=□Cu, Ag, Au) on CeO2 (100) surface. *Journal of Power Sources*, **2013**, 234, 69-81	8.9	27
122	Is silicene stable in O 2 ? □irst-principles study of O 2 dissociation and O 2 -dissociation□nduced oxygen atoms adsorption on free-standing silicene. *Europhysics Letters*, **2014**, 106, 47001	1.6	26
121	First principles study of wurtzite and zinc blende GaN: a comparison of the electronic and optical properties. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2005**, 336, 145-151	2.3	26
120	Ab initio studies on the stability and electronic structure of LiCoO2 (003) surfaces. *Physical Review B*, **2005**, 71,	3.3	25
119	Surface Modification of the LiNiCoMnO Cathode Material by Coating with FePO with a Yolk-Shell Structure for Improved Electrochemical Performance. *ACS Applied Materials & Interfaces*, **2020**, 12, 36046-36053	9.5	25
118	O-vacancy and surface on CeO2: A first-principles study. *Journal of Physics and Chemistry of Solids*, **2010**, 71, 788-796	3.9	24
117	Improving the electrical conductivity and structural stability of the Li 2 MnO 3 cathode via P doping. *Journal of Alloys and Compounds*, **2016**, 658, 818-823	5.7	23

116	Lithium ion adsorption and diffusion on black phosphorene nanotube: A first-principles study. *Applied Surface Science*, **2017**, 392, 88-94	6.7	23
115	Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. *National Science Review*, **2020**, 7, 1768-1775	10.8	23
114	The structural and electronic properties of spinel MnCo2O4 bulk and low-index surfaces: From first principles studies. *Applied Surface Science*, **2015**, 349, 510-515	6.7	22
113	Tuning the electronic properties of germanene by molecular adsorption and under an external electric field. *Journal of Materials Chemistry C*, **2018**, 6, 5937-5948	7.1	22
112	First-Principles Calculation of Lithium Adsorption and Diffusion on Silicene. *Chinese Physics Letters*, **2013**, 30, 017103	1.8	22
111	Role of alloying elements in vanadium-based binary alloy membranes for hydrogen separation. *Journal of Membrane Science*, **2012**, 423-424, 332-341	9.6	22
110	The role of Cu in degrading adsorption of CO on the PtnCu clusters. *Journal of Physical Chemistry A*, **2013**, 117, 8293-7	2.8	21
109	Experimental and theoretical studies on dynamic properties of Li ions in LixMn2O4. *Solid State Communications*, **2004**, 130, 501-506	1.6	21
108	Formation and thermodynamic stability of oxygen vacancies in typical cathode materials for Li-ion batteries: Density functional theory study. *Solid State Ionics*, **2020**, 347, 115257	3.3	20
107	Theoretical prediction of T-graphene as a promising alkali-ion battery anode offering ultrahigh capacity. *Physical Chemistry Chemical Physics*, **2020**, 22, 3281-3289	3.6	20
106	Insight into the Vibrational and Thermodynamic Properties of Layered Lithium Transition-Metal Oxides LiMO2 (M = Co, Ni, Mn): A First-Principles Study. *Journal of Physical Chemistry C*, **2016**, 120, 5876-5882	3.8	20
105	Physics towards next generation Li secondary batteries materials: A short review from computational materials design perspective. *Science China: Physics, Mechanics and Astronomy*, **2013**, 56, 2278-2292	3.6	20
104	STRAIN INDUCED ENHANCED MIGRATION OF POLARON AND LITHIUM ION IN □MnO2. *Functional Materials Letters*, **2012**, 05, 1250037	1.2	20
103	Multi-scale stabilization of high-voltage LiCoO2 enabled by nanoscale solid electrolyte coating. *Energy Storage Materials*, **2020**, 29, 71-77	19.4	19
102	Hydrogen storage on calcium-decorated BC7 sheet: A first-principles study. *International Journal of Hydrogen Energy*, **2014**, 39, 2142-2148	6.7	19
101	First-principles study of lithium intercalated bilayer graphene. *Science China: Physics, Mechanics and Astronomy*, **2012**, 55, 1376-1382	3.6	19
100	Understanding the effect of the layer-to-layer distance on Li-intercalated graphite. *Journal of Applied Physics*, **2012**, 111, 124325	2.5	19
99	Pulsed laser deposition prepared LiMn 2 O 4 thin film. *Thin Solid Films*, **2006**, 503, 268-271	2.2	19

98	Ab initio investigation of Jahn□Teller-distortion-tuned Li-ion migration in □MnO2. *Journal of Materials Chemistry A*, **2017**, 5, 9618-9626	13	18
97	Na2MnO3 as cathode materials for Na ion batteries: From first-principles investigations. *Solid State Ionics*, **2018**, 320, 210-214	3.3	18
96	Comparison of the stability of free-standing silicene and hydrogenated silicene in oxygen: a first principles investigation. *Journal of Physics Condensed Matter*, **2014**, 26, 355007	1.8	18
95	Transition from Mn(4+) to Mn(3+) induced by surface reconstruction at □MnO(2)(001). *Journal of Chemical Physics*, **2010**, 133, 204701	3.9	18
94	Cobalt suppressed Jahn□Teller effect in LiCo0.5Ni0.5O2 for lithium ion batteries. *Solid State Communications*, **2011**, 151, 234-237	1.6	18
93	A first-principles investigation of Janus MoSSe as a catalyst for photocatalytic water-splitting. *Applied Surface Science*, **2021**, 537, 147919	6.7	17
92	Organosilicon functionalized glycerol carbonates as electrolytes for lithium-ion batteries. *RSC Advances*, **2015**, 5, 17660-17666	3.7	16
91	Polaron states and migration in F-doped Li2MnO3. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2449-2452	2.3	16
90	Li1+xFePO4 (0□□) as anode material for lithium ion batteries: From ab initio studies. *Journal of Power Sources*, **2008**, 175, 891-896	8.9	16
89	Comparisons between adsorption and diffusion of alkali, alkaline earth metal atoms on silicene and those on silicane: Insight from first-principles calculations. *Chinese Physics B*, **2016**, 25, 067103	1.2	15
88	Density functional theory study of Ir atom deposited on □Al2O3 (001) surface. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 277-281	2.3	15
87	Electronic structure and magnetism of EuX (X = O, S, Se and Te): A first-principles investigation. *Europhysics Letters*, **2008**, 83, 69001	1.6	15
86	First-principles study on electronic structure of LiFePO4. *Solid State Communications*, **2007**, 143, 144-148	1.6	15
85	The effect of strain on band structure of single-layer MoS2: an ab initio study. *Wuli Xuebao/Acta Physica Sinica*, **2012**, 61, 227102	0.6	15
84	The adsorption and dissociation of oxygen on Ag (111) supported □3 borophene. *Physica B: Condensed Matter*, **2018**, 537, 1-6	2.8	14
83	First-principles study of the stability of free-standing germanene in oxygen atmosphere. *Journal of Applied Physics*, **2015**, 118, 124303	2.5	14
82	Jahn□Teller type small polaron assisted Na diffusion in NaMnO2 as a cathode material for Na-ion batteries. *Journal of Materials Chemistry A*, **2019**, 7, 6053-6061	13	14
81	First Principles Study of Penta-siligraphene as High-Performance Anode Material for Li-Ion Batteries. *Nanoscale Research Letters*, **2019**, 14, 260	5	13

80	Insights into the physics of interaction between borophene and O2-first-principles investigation. *Computational Materials Science*, **2017**, 140, 261-266	3.2	13
79	First-principles study on the electronic structures of Cr- and W-doped single-layer MoS2. *Wuli Xuebao/Acta Physica Sinica*, **2013**, 62, 037103	0.6	13
78	The effect of protons on the Mg migration in an □VO cathode for magnesium batteries: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2019**, 21, 7406-7411	3.6	12
77	The effect of titanium(Ti) doping on hydrogen incorporation in tungsten(W):First-principles calculations. *Fusion Engineering and Design*, **2017**, 121, 227-234	1.7	12
76	First principles study of g-MgN as an anode material for Na-, K-, Mg-, Ca- and Al-ion storage.. *RSC Advances*, **2019**, 9, 27378-27385	3.7	11
75	2D honeycomb borophene oxide: a promising anode material offering super high capacity for Li/Na-ion batteries. *Journal of Physics Condensed Matter*, **2020**, 32, 065001	1.8	11
74	First principles study of alkali and alkaline earth metal ions adsorption and diffusion on penta-graphene. *Solid State Ionics*, **2019**, 342, 115062	3.3	11
73	First-Principles Study of Lithium and Sodium Atoms Intercalation in Fluorinated Graphite. *Engineering*, **2015**, 1, 243-246	9.7	11
72	Hydrogen solution in tetrahedral or octahedral interstitial sites in Al. *Journal of Alloys and Compounds*, **2011**, 509, 9214-9217	5.7	11
71	Preparation and temperature-dependent photoluminescence properties of ScF3:Eu3+ submicroparticles. *New Journal of Chemistry*, **2017**, 41, 7915-7923	3.6	10
70	New insights into Li diffusion in Li-Si alloys for Si anode materials: role of Si microstructures. *Nanoscale*, **2019**, 11, 14042-14049	7.7	10
69	Calcium Doping of Lithium Titanium Oxide Nanospheres: A Combined First-Principles and Experimental Study. *Energy Technology*, **2017**, 5, 539-543	3.5	10
68	Iodine ion transport in solid electrolyte LiI(C3H5NO)2: a first-principles identification. *Ionics*, **2007**, 12, 343-347	2.7	10
67	Confined Li ion migration in the silicon-graphene complex system: An ab initio investigation. *Applied Surface Science*, **2018**, 436, 505-510	6.7	10
66	Density functional theory prediction of MgN as a high-performance anode material for Li-ion batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 7053-7060	3.6	9
65	First-principles identification of spinel CaCo2O4 as a promising cathode material for Ca-ion batteries. *Solid State Ionics*, **2018**, 326, 145-149	3.3	9
64	Compressive strain induced dynamical stability of monolayer 1T-MX2 (M = Mo, W; X = S, Se). *Materials Research Express*, **2017**, 4, 115018	1.7	8
63	Manipulation of spin-flip in Co3O4: a first principles study. *Journal of Materials Science*, **2016**, 51, 4691-4696	4.5	8

62	The structural, mechanical and electronic properties of (4,4) SiC/C nanotube heterojunction: A first-principles study. *Computational Materials Science*, **2013**, 68, 367-370	3.2	8
61	Time dependence of the average charge and current in a dissipative mesoscopic circuit. *Chinese Physics B*, **2002**, 11, 163-166		8
60	Effect of Interstitial Hydrogen on the Mechanical and Thermal Properties of Tungsten: A First-Principles Study. *Journal of Physical Chemistry C*, **2019**, 123, 1913-1921	3.8	8
59	Further discussions on the geometry and fast diffusion of AlCl4 cluster intercalated in graphite. *Electrochimica Acta*, **2017**, 223, 137-139	6.7	7
58	The structural and electronic properties of Pt-Cu alloy clusters: Embedding atom method combined with density functional theory study. *Journal of Alloys and Compounds*, **2018**, 741, 604-609	5.7	7
57	Facile microwave synthesis of ScPO4□2H2O flowerlike superstructures: morphology control, electronic structure and multicolor tunable luminescent properties. *CrystEngComm*, **2017**, 19, 5787-5796	3.3	7
56	First principles studies on the electronic structures of Li M x Fe 1-x PO 4 (M = Co, Ni and Rh). *Chinese Physics B*, **2007**, 16, 3042-3045		6
55	Shapiro effect in mesoscopic LC circuit. *Chinese Physics B*, **2002**, 11, 720-724		6
54	Interpenetrating graphene network bct-C: a promising anode material for Li ion batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 23485-23491	3.6	6
53	Scandium Molybdate Microstructures with Tunable Phase and Morphology: Microwave Synthesis, Theoretical Calculations, and Photoluminescence Properties. *Inorganic Chemistry*, **2019**, 58, 2491-2500	5.1	6
52	Electron-donor doping enhanced Li storage in electride CaN monolayer: a first-principles study. *Journal of Physics Condensed Matter*, **2018**, 30, 345501	1.8	5
51	The stability of free-standing germanane in oxygen: First-principles investigation. *Europhysics Letters*, **2015**, 110, 17007	1.6	5
50	First-principles study on the electronic structures of □SiC/carbon nanotube core-shell structures. *Wuli Xuebao/Acta Physica Sinica*, **2013**, 62, 107101	0.6	5
49	First principles investigation of dynamic performance in the process of lithium intercalation into black phosphorus. *Wuli Xuebao/Acta Physica Sinica*, **2012**, 61, 247101	0.6	5
48	LiGaOS is a fast Li-Ion conductor: A first-principles prediction. *Materials and Design*, **2020**, 185, 108264	8.1	5
47	Electric-field-tunable molecular adsorption on germanane. *Physical Chemistry Chemical Physics*, **2019**, 21, 20287-20295	3.6	4
46	First-principles study on the structural, electronic, and Li-ion mobility properties of anti-perovskite superionic conductor Li3OCl (1□0) surface. *Applied Surface Science*, **2020**, 510, 145394	6.7	4
45	Highly optimized embedding atom method potential for Pt-Cu alloys. *Journal of Alloys and Compounds*, **2017**, 696, 470-480	5.7	4

44	Hydrogen solution in tungsten (W) under different temperatures and strains: a first principles calculation study. *Physical Chemistry Chemical Physics*, **2020**, 22, 19623-19630	3.6	4
43	The strain effect on lithium ion migration in Li-Si alloys: A first-principles study. *Solid State Communications*, **2016**, 247, 47-52	1.6	4
42	The effect of titanium doping on carbon behavior in tungsten: A first-principles study. *Fusion Engineering and Design*, **2016**, 112, 123-129	1.7	4
41	Bonding interactions in Li/Na oxides, peroxides and superoxides and their implication to the performance of the Li/Na-air batteries. *Solid State Ionics*, **2017**, 303, 24-28	3.3	3
40	Structural and Electronic Features of Nb-Doped SrCoO3: Insight from First-Principles Calculations. *Journal of Physical Chemistry C*, **2017**, 121, 24987-24993	3.8	3
39	Dissociation of (LiO) on graphene and boron-doped graphene: insights from first-principles calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 14216-14224	3.6	3
38	First-principles study of borophene for charge-modulated switchable CO capture. *Physical Chemistry Chemical Physics*, **2020**, 22, 8864-8869	3.6	3
37	Effects of hydrogen on Mn-doped GaN: A first principles calculation. *Physica B: Condensed Matter*, **2013**, 425, 38-41	2.8	3
36	Vacancy and H Interactions in Nb. *Chinese Physics Letters*, **2011**, 28, 127101	1.8	3
35	Insights into Bulk Properties and Transport Mechanisms in New Ternary Halide Solid Electrolytes: First-Principles Calculations. *Journal of Physical Chemistry C*, **2021**, 125, 23510-23520	3.8	3
34	Effects of Strain and Electric Field on Molecular Doping in MoSSe. *ACS Omega*, **2021**, 6, 14639-14647	3.9	3
33	Structural, electronic, sodium diffusion and elastic properties of NaP alloy anode for Na-ion batteries: Insight from first-principles calculations. *Modern Physics Letters B*, **2016**, 30, 1650385	1.6	3
32	A novel organosilicon-based ionic plastic crystal as solid-state electrolyte for lithium-ion batteries. *Journal of Zhejiang University: Science A*, **2016**, 17, 155-162	2.1	3
31	Comparative study on dynamical stability against strain of pristine and chemically functionalized monolayer honeycomb materials. *Journal of Materials Science*, **2018**, 53, 4306-4315	4.3	3
30	Strain-tunable molecular doping in germanane: a first-principles study. *Nanotechnology*, **2018**, 29, 465202	3.4	3
29	Design and Properties Prediction of AMCOF by First-Principles Calculations. *ACS Applied Materials & Interfaces*, **2017**, 9, 13255-13261	9.5	2
28	Li ion diffusion dynamics on Li oxides and peroxides surfaces. *Materials Letters*, **2017**, 188, 208-211	3.3	2
27	Jahn–Teller distortion affected Li ion migration in spinel TiO2. *Solid State Ionics*, **2017**, 312, 17-20	3.3	2

26	Phosphorus-Mediated MoS2: Phosphorus-Mediated MoS2 Nanowires as a High-Performance Electrode Material for Quasi-Solid-State Sodium-Ion Intercalation Supercapacitors (Small 4/2019). *Small*, **2019**, 15, 1970026	11	2
25	The effect of strain on the Li-storage performance of V2C and Nb2C: From first-principles study. *Solid State Communications*, **2020**, 311, 113857	1.6	2
24	First principle study of Li X S 2 (X = Ga, In) as cathode materials for Li ion batteries. *Chinese Physics B*, **2016**, 25, 028202	1.2	2
23	Curvature induced improvement of Li storage in Ca2N nanotubes. *Applied Surface Science*, **2018**, 459, 406-410	6.7	2
22	Structural and electronic properties of small lithium peroxide clusters in view of the charge process in Li-O batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 19935-19943	3.6	2
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