Chuying Ouyang

List of Publications by Year in Descending Order

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

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	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
186	Two-dimensional MnN utilized as high-capacity anode for Li-ion batteries*. *Chinese Physics B*, **2021**, 30, 046302	1.2	1
185	Effects of Strain and Electric Field on Molecular Doping in MoSSe. *ACS Omega*, **2021**, 6, 14639-14647	3.9	3
184	First-principles calculation identification of ultrahigh hydrogen storage capacity in g-Mg3N2. *Journal of Alloys and Compounds*, **2021**, 867, 158744	5.7	1
183	A first-principles investigation of Janus MoSSe as a catalyst for photocatalytic water-splitting. *Applied Surface Science*, **2021**, 537, 147919	6.7	17
182	Adsorption of propylene carbonate on the LiMn2O4 (100) surface investigated by DFT + U calculations*. *Chinese Physics B*, **2021**, 30, 038202	1.2	1
181	The thermodynamics and electronic structure analysis of P-doped spinel CoO. *Physical Chemistry Chemical Physics*, **2021**, 23, 3588-3594	3.6	1
180	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
179	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
178	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
177	An Sc-based coordination polymer with concaved superstructures: preparation, formation mechanism, conversion, and their electrochemistry properties. *CrystEngComm*, **2020**, 22, 2926-2932	3.3	
176	First-principles study of □borophene for charge-modulated switchable CO capture. *Physical Chemistry Chemical Physics*, **2020**, 22, 8864-8869	3.6	3
175	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
174	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
173	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
172	The effect of thickness on the Li-ion adsorption behaviors of 2D Ti1C multi-layers from first-principles calculations. *Thin Solid Films*, **2020**, 704, 138019	2.2	0
171	Multi-scale stabilization of high-voltage LiCoO2 enabled by nanoscale solid electrolyte coating. *Energy Storage Materials*, **2020**, 29, 71-77	19.4	19

170	Structural and Electronic Properties of Small Stoichiometric (Li2O2)n Clusters and Relevance to Li□2 Batteries. *Journal of Cluster Science*, **2020**, 31, 643-649	3	1
169	Strong Jahn-Teller effect at NiO4 tetrahedron in NiCo2O4 spinel. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126114	2.3	0
168	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
167	First-principles insights of hydrogen diffusion dynamics at the □Al2O3 (0001) surface. *Applied Surface Science*, **2020**, 531, 147263	6.7	1
166	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
165	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
164	LiGaOS is a fast Li-Ion conductor: A first-principles prediction. *Materials and Design*, **2020**, 185, 108264	8.1	5
163	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
162	Electric-field-tunable molecular adsorption on germanane. *Physical Chemistry Chemical Physics*, **2019**, 21, 20287-20295	3.6	4
161	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
160	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
159	Germagraphene as a promising anode material for lithium-ion batteries predicted from first-principles calculations. *Nanoscale Horizons*, **2019**, 4, 457-463	10.8	36
158	Trace doping of multiple elements enables stable battery cycling of LiCoO2 at 4.6 V. *Nature Energy*, **2019**, 4, 594-603	62.3	299
157	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
156	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
155	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
154	First Principles Study of Penta-siligraphene as High-Performance Anode Material for Li-Ion Batteries. *Nanoscale Research Letters*, **2019**, 14, 260	5	13
153	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

152	First-principles study of rare-earth-doped cathode materials Li2MnO3 in Li-ion batteries. *Wuli Xuebao/Acta Physica Sinica*, **2019**, 68, 138201	0.6	1
151	First-principles study of reduction mechanism of oxygen molecule using nitrogen doped graphene as cathode material for lithium air batteries. *Wuli Xuebao/Acta Physica Sinica*, **2019**, 68, 128801	0.6	2
150	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
149	Jahn□eller 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
148	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
147	Interpenetrating graphene network bct-C: a promising anode material for Li ion batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 23485-23491	3.6	6
146	Three-dimensional honeycomb carbon: Junction line distortion and novel emergent fermions. *Carbon*, **2019**, 141, 417-426	10.4	29
145	Phosphorus-Mediated MoS Nanowires as a High-Performance Electrode Material for Quasi-Solid-State Sodium-Ion Intercalation Supercapacitors. *Small*, **2019**, 15, e1803984	11	54
144	Tailoring Lithium Deposition via an SEI-Functionalized Membrane Derived from LiF Decorated Layered Carbon Structure. *Advanced Energy Materials*, **2019**, 9, 1802912	21.8	74
143	Scandium Molybdate Microstructures with Tunable Phase and Morphology: Microwave Synthesis, Theoretical Calculations, and Photoluminescence Properties. *Inorganic Chemistry*, **2019**, 58, 2491-2500	5.1	6
142	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
141	Phosphorous-containing oxygen-deficient cobalt molybdate as an advanced electrode material for supercapacitors. *Energy Storage Materials*, **2019**, 19, 186-196	19.4	90
140	Molecular adsorption and strain-induced ferromagnetic semiconductor-metal transition in half-hydrogenated germanene. *Journal of Applied Physics*, **2019**, 125, 082504	2.5	1
139	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
138	Siligraphene as a promising anode material for lithium-ion batteries predicted from first-principles calculations. *Nano Energy*, **2018**, 49, 67-76	17.1	65
137	The adsorption and dissociation of oxygen on Ag (111) supported □B borophene. *Physica B: Condensed Matter*, **2018**, 537, 1-6	2.8	14
136	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
135	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

134	Na2MnO3 as cathode materials for Na ion batteries: From first-principles investigations. *Solid State Ionics*, **2018**, 320, 210-214	3.3	18
133	Bandgap tuning in MoSSe bilayers: synergistic effects of dipole moment and interlayer distance. *Physical Chemistry Chemical Physics*, **2018**, 20, 20919-20926	3.6	32
132	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
131	Curvature induced improvement of Li storage in Ca2N nanotubes. *Applied Surface Science*, **2018**, 459, 406-410	6.7	2
130	Confined Li ion migration in the silicon-graphene complex system: An ab initio investigation. *Applied Surface Science*, **2018**, 436, 505-510	6.7	10
129	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
128	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
127	Ab initio molecular dynamics simulation of irradiation particles behavior in tungsten. *European Physical Journal B*, **2018**, 91, 1	1.2	
126	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
125	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
124	Strain-tunable molecular doping in germanane: a first-principles study. *Nanotechnology*, **2018**, 29, 465202	3.4	3
123	Further discussions on the geometry and fast diffusion of AlCl4 cluster intercalated in graphite. *Electrochimica Acta*, **2017**, 223, 137-139	6.7	7
122	Design and Properties Prediction of AMCOF by First-Principles Calculations. *ACS Applied Materials & Interfaces*, **2017**, 9, 13255-13261	9.5	2
121	Ab initio investigation of Jahn□Teller-distortion-tuned Li-ion migration in □MnO2. *Journal of Materials Chemistry A*, **2017**, 5, 9618-9626	13	18
120	Preparation and temperature-dependent photoluminescence properties of ScF3:Eu3+ submicroparticles. *New Journal of Chemistry*, **2017**, 41, 7915-7923	3.6	10
119	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
118	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
117	Li ion diffusion dynamics on Li oxides and peroxides surfaces. *Materials Letters*, **2017**, 188, 208-211	3.3	2

116	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
115	Compressive strain induced dynamical stability of monolayer 1T-MX2 (M = Mo, W; X = S, Se). *Materials Research Express*, **2017**, 4, 115018	1.7	8
114	Jahn□eller distortion affected Li ion migration in spinel TiO2. *Solid State Ionics*, **2017**, 312, 17-20	3.3	2
113	Insights into the physics of interaction between borophene and O2-first-principles investigation. *Computational Materials Science*, **2017**, 140, 261-266	3.2	13
112	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
111	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
110	Calcium Doping of Lithium Titanium Oxide Nanospheres: A Combined First-Principles and Experimental Study. *Energy Technology*, **2017**, 5, 539-543	3.5	10
109	Lithium ion adsorption and diffusion on black phosphorene nanotube: A first-principles study. *Applied Surface Science*, **2017**, 392, 88-94	6.7	23
108	Highly optimized embedding atom method potential for Pt-Cu alloys. *Journal of Alloys and Compounds*, **2017**, 696, 470-480	5.7	4
107	Mechanical properties of W□i alloys from first-principles calculations. *Fusion Engineering and Design*, **2016**, 106, 34-39	1.7	29
106	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
105	Coordination of lithium ion with ethylene carbonate electrolyte solvent: A computational study. *International Journal of Quantum Chemistry*, **2016**, 116, 97-102	2.1	29
104	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
103	Multi-scale computation methods: Their applications in lithium-ion battery research and development. *Chinese Physics B*, **2016**, 25, 018212	1.2	346
102	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
101	Physics of electron and lithium-ion transport in electrode materials for Li-ion batteries. *Chinese Physics B*, **2016**, 25, 018206	1.2	27
100	Manipulation of spin-flip in Co3O4: a first principles study. *Journal of Materials Science*, **2016**, 51, 4691-4696	4.5	8
99	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

98	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
97	Geometry and fast diffusion of AlCl4 cluster intercalated in graphite. *Electrochimica Acta*, **2016**, 195, 158-165	6.7	69
96	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
95	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
94	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
93	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
92	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
91	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
90	Structural Features of Medium-Sized Ge n (n = 35, 40, 45, 50, 55 and 60) clusters. *Journal of Cluster Science*, **2015**, 26, 1001-1010	3	1
89	Organosilicon functionalized glycerol carbonates as electrolytes for lithium-ion batteries. *RSC Advances*, **2015**, 5, 17660-17666	3.7	16
88	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
87	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
86	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
85	First-principles study of the stability of free-standing germanene in oxygen atmosphere. *Journal of Applied Physics*, **2015**, 118, 124303	2.5	14
84	First-Principles Study of Lithium and Sodium Atoms Intercalation in Fluorinated Graphite. *Engineering*, **2015**, 1, 243-246	9.7	11
83	The stability of free-standing germanane in oxygen: First-principles investigation. *Europhysics Letters*, **2015**, 110, 17007	1.6	5
82	W6+ & Br□odoped Li4Ti5O12 anode with super rate performance for Li-ion batteries. *Journal of Materials Chemistry A*, **2015**, 3, 13706-13716	13	59
81	Nitrogen- and Phosphorus-Doped Biocarbon with Enhanced Electrocatalytic Activity for Oxygen Reduction. *ACS Catalysis*, **2015**, 5, 920-927	13.1	124

80	Hydrogen storage on calcium-decorated BC7 sheet: A first-principles study. *International Journal of Hydrogen Energy*, **2014**, 39, 2142-2148	6.7	19
79	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
78	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
77	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
76	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
75	Curvature induced magnetic nanonodes in (6, 0) SiC/C nanotube heterojunction superlattice. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 58, 153-156	3	1
74	Insights into structural stability and Li superionic conductivity of Li10GeP2S12 from first-principles calculations. *Chemical Physics Letters*, **2014**, 591, 16-20	2.5	28
73	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
72	Is silicene stable in O 2 ? First-principles study of O 2 dissociation and O 2 -dissociation induced oxygen atoms adsorption on free-standing silicene. *Europhysics Letters*, **2014**, 106, 47001	1.6	26
71	Effect of strain on Li adsorption on silicene. *Wuli Xuebao/Acta Physica Sinica*, **2014**, 63, 217101	0.6	1
70	First-Principles Calculation of Lithium Adsorption and Diffusion on Silicene. *Chinese Physics Letters*, **2013**, 30, 017103	1.8	22
69	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
68	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
67	Effects of hydrogen on Mn-doped GaN: A first principles calculation. *Physica B: Condensed Matter*, **2013**, 425, 38-41	2.8	3
66	STRAIN-TUNABLE BAND GAP OF BC3 SHEET: A FIRST-PRINCIPLES INVESTIGATION. *Modern Physics Letters B*, **2013**, 27, 1350110	1.6	2
65	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
64	The Origin of BC 7 Sheet Metallicity and the Tuning of its Electronic Properties by Hydrogenation. *Chinese Physics Letters*, **2013**, 30, 066102	1.8	2
63	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

62	STRUCTURAL AND ELECTRONIC EVOLUTION FROM SiC SHEET TO SILICENE. *International Journal of Modern Physics B*, **2013**, 27, 1350188	1.1	2
61	FIRST-PRINCIPLES STUDY ON β-SiC/BNNT CORE/SHELL NANOCABLE. *Modern Physics Letters B*, **2013**, 27, 1350169	1.6	
60	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
59	First-principles study on the electronic structures of β-SiC/carbon nanotube core-shell structures. *Wuli Xuebao/Acta Physica Sinica*, **2013**, 62, 107101	0.6	5
58	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
57	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
56	Synthesis and Lithium Storage Mechanism of Ultrafine MoO2 Nanorods. *Chemistry of Materials*, **2012**, 24, 457-463	9.6	201
55	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
54	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
53	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
52	Strain-induced semimetal-metal transition in silicene. *Europhysics Letters*, **2012**, 99, 17010	1.6	70
51	First-principles study of lithium intercalated bilayer graphene. *Science China: Physics, Mechanics and Astronomy*, **2012**, 55, 1376-1382	3.6	19
50	STRAIN INDUCED ENHANCED MIGRATION OF POLARON AND LITHIUM ION IN β-MnO2. *Functional Materials Letters*, **2012**, 05, 1250037	1.2	20
49	Understanding the effect of the layer-to-layer distance on Li-intercalated graphite. *Journal of Applied Physics*, **2012**, 111, 124325	2.5	19
48	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
47	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
46	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
45	Hydrogen solution in tetrahedral or octahedral interstitial sites in Al. *Journal of Alloys and Compounds*, **2011**, 509, 9214-9217	5.7	11

44	Hydrogen-induced interactions in vanadium from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	44
43	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
42	Lithium ion diffusion in Li4+xTi5O12: From ab initio studies. *Electrochimica Acta*, **2011**, 56, 6084-6088	6.7	44
41	Cobalt suppressed Jahn□Teller effect in LiCo0.5Ni0.5O2 for lithium ion batteries. *Solid State Communications*, **2011**, 151, 234-237	1.6	18
40	Vacancy and H Interactions in Nb. *Chinese Physics Letters*, **2011**, 28, 127101	1.8	3
39	Improving the Electrochemical Activity of LiMnPO[sub 4] Via Mn-Site Substitution. *Journal of the Electrochemical Society*, **2010**, 157, A225	3.9	98
38	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
37	First-principles investigation on redox properties of M-doped CeO2 (M=Mn,Pr,Sn,Zr). *Physical Review B*, **2010**, 82,	3.3	100
36	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
35	Ab initio studies on atomic and electronic structures of black phosphorus. *Journal of Applied Physics* , **2010**, 107, 093718	2.5	200
34	O-vacancy and surface on CeO2: A first-principles study. *Journal of Physics and Chemistry of Solids*, **2010**, 71, 788-796	3.9	24
33	First principles studies on the structural and electronic properties of Srn+1TinO3n+1 (n=1, 2, 3, ∞) *Physica B: Condensed Matter*, **2010**, 405, 4780-4784	2.8	1
32	First principles study of Jahn□Teller effects in LixMnPO4. *Solid State Communications*, **2010**, 150, 40-44	1.6	76
31	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
30	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
29	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
28	First-principles investigation of the bonding, optical and lattice dynamical properties of CeO2. *Journal of Power Sources*, **2009**, 194, 830-834	8.9	43
27	First-principles study of □Al2O3 (100) surface. *Physical Review B*, **2009**, 79,	3.3	34

26	Jahn□Teller distortion and electronic structure of LiMn2O4. *Journal of Alloys and Compounds*, **2009**, 474, 370-374	5.7	133
25	Electronic structure and magnetism of EuX (X = O, S, Se and Te): A first-principles investigation. *Europhysics Letters*, **2008**, 83, 69001	1.6	15
24	Li1+xFePO4 (0□□3) as anode material for lithium ion batteries: From ab initio studies. *Journal of Power Sources*, **2008**, 175, 891-896	8.9	16
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