Chuying Ouyang

List of Publications by Year in descending order

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189 papers	9,181 citations	43973 48 h-index	45213 90 g-index
191 all docs	191 docs citations	191 times ranked	10169 citing authors

#	Article	IF	Citations
1	Trace doping of multiple elements enables stable battery cycling of LiCoO2 at 4.6â€‰V. Nature Energy, 2019, 4, 594-603.	19.8	572
2	Multi-scale computation methods: Their applications in lithium-ion battery research and development. Chinese Physics B, 2016, 25, 018212.	0.7	449
3	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.	6.6	303
4	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.	1.5	301
5	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.	5.2	266
6	Ab initio studies of structural and electronic properties of Li4Ti5O12 spinel. Electrochemistry Communications, 2007, 9, 1107-1112.	2.3	265
7	First-principles study of Li ion diffusion inLiFePO4. Physical Review B, 2004, 69, .	1.1	250
8	Enhancement of electronic conductivity ofLiFePO4by Cr doping and its identification by first-principles calculations. Physical Review B, 2003, 68, .	1.1	249
9	Ab initio studies on atomic and electronic structures of black phosphorus. Journal of Applied Physics, 2010, 107, .	1.1	235
10	Synthesis and Lithium Storage Mechanism of Ultrafine MoO₂ Nanorods. Chemistry of Materials, 2012, 24, 457-463.	3.2	230
11	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.	9.5	189
12	2D Electrides as Promising Anode Materials for Na-Ion Batteries from First-Principles Study. ACS Applied Materials & Interfaces, 2015, 7, 24016-24022.	4.0	181
13	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.	1.5	179
14	Jahnâ€“Teller distortion and electronic structure of LiMn2O4. Journal of Alloys and Compounds, 2009, 474, 370-374.	2.8	169
15	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.	1.7	147
16	Phosphorous-containing oxygen-deficient cobalt molybdate as an advanced electrode material for supercapacitors. Energy Storage Materials, 2019, 19, 186-196.	9.5	145
17	Nitrogen- and Phosphorus-Doped Biocarbon with Enhanced Electrocatalytic Activity for Oxygen Reduction. ACS Catalysis, 2015, 5, 920-927.	5.5	139
18	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, .	1.1	133

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19	Effect of Co Content on Rate Performance of LiMn[sub 0.5â^'x]Co[sub 2x]Ni[sub 0.5â^'x]O[sub 2] Cathode Materials for Lithium-Ion Batteries. Journal of the Electrochemical Society, 2004, 151, A504.	1.3	129
20	Improving the Electrochemical Activity of LiMnPO[sub 4] Via Mn-Site Substitution. Journal of the Electrochemical Society, 2010, 157, A225.	1.3	112
21	First-principles investigation on redox properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>M</mml:mi></mml:math>-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CeO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>	1.1	112
22	Ab initio Studies on Li_{4+x}Ti₅O₁₂ Compounds as Anode Materials for Lithiumâ€Ion Batteries. ChemPhysChem, 2008, 9, 2104-2108.	1.0	110
23	Tailoring Lithium Deposition via an SEIâ€Functionalized Membrane Derived from LiF Decorated Layered Carbon Structure. Advanced Energy Materials, 2019, 9, 1802912.	10.2	98
24	First principles study of Jahnâ€“Teller effects in LixMnPO4. Solid State Communications, 2010, 150, 40-44.	0.9	95
25	Siligraphene as a promising anode material for lithium-ion batteries predicted from first-principles calculations. Nano Energy, 2018, 49, 67-76.	8.2	95
26	Strain tuned Li diffusion in LiCoO2 material for Li ion batteries: A first principles study. Solid State Ionics, 2014, 263, 46-48.	1.3	92
27	First-principles study of high-capacity hydrogen storage on graphene with Li atoms. Journal of Physics and Chemistry of Solids, 2012, 73, 245-251.	1.9	88
28	Geometry and fast diffusion of AlCl4 cluster intercalated in graphite. Electrochimica Acta, 2016, 195, 158-165.	2.6	84
29	Theoretical study of cation doping effect on the electronic conductivity of Li4Ti5O12. Physica Status Solidi (B): Basic Research, 2006, 243, 1835-1841.	0.7	83
30	Phosphorusâ€Mediated MoS₂ Nanowires as a Highâ€Performance Electrode Material for Quasiâ€Solidâ€State Sodiumâ€Ion Intercalation Supercapacitors. Small, 2019, 15, e1803984.	5.2	81
31	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.	0.7	79
32	Effect of Mg-doping on the structural and electronic properties of LiCoO2: A first-principles investigation. Journal of Power Sources, 2007, 171, 908-912.	4.0	79
33	Strain-induced semimetal-metal transition in silicene. Europhysics Letters, 2012, 99, 17010.	0.7	75
34	Oxidation States of Mn Atoms at Clean and Al₂O₃-Covered LiMn₂O₄(001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 4756-4759.	1.5	73
35	W⁶⁺ & Br^{â^'} codoped Li₄Ti₅O₁₂ anode with super rate performance for Li-ion batteries. Journal of Materials Chemistry A, 2015, 3, 13706-13716.	5.2	73
36	Tunable electronic structures in BP/MoSSe van der Waals heterostructures by external electric field and strain. Applied Surface Science, 2019, 497, 143809.	3.1	71

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37	Li-decorated graphyne as high-capacity hydrogen storage media: First-principles plane wave calculations. International Journal of Hydrogen Energy, 2014, 39, 17104-17111.	3.8	67
38	Ce 3+ -doped Li 4 Ti 5 O 12 with CeO 2 surface modification by a sol-gel method for high-performance lithium-ion batteries. Electrochimica Acta, 2016, 189, 147-157.	2.6	66
39	Surface Modification of the LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂ Cathode Material by Coating with FePO₄ with a Yolkâ€“Shell Structure for Improved Electrochemical Performance. ACS Applied Materials & Interfaces, 2020, 12, 36046-36053.	4.0	58
40	First-principles investigation of the structural, magnetic, and electronic properties of olivineLiFePO4. Physical Review B, 2005, 71, .	1.1	57
41	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.	0.7	56
42	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.	5.2	56
43	Theoretical Prediction of Janus MoSSe as a Potential Anode Material for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 23899-23909.	1.5	56
44	First-principles investigation of the bonding, optical and lattice dynamical properties of CeO2. Journal of Power Sources, 2009, 194, 830-834.	4.0	54
45	The effect of cation doping on spinel LiMn2O4: a first-principles investigation. Solid State Communications, 2003, 126, 531-534.	0.9	52
46	First-principles investigation of transition metal atom M (M = Cu, Ag, Au) adsorption on CeO2(110). Physical Chemistry Chemical Physics, 2012, 14, 1923.	1.3	52
47	Theoretical prediction of T-graphene as a promising alkali-ion battery anode offering ultrahigh capacity. Physical Chemistry Chemical Physics, 2020, 22, 3281-3289.	1.3	51
48	First Principles Study on Na x Li 1â^' x FePO 4 As Cathode Material for Rechargeable Lithium Batteries. Chinese Physics Letters, 2006, 23, 61-64.	1.3	49
49	Multi-scale stabilization of high-voltage LiCoO2 enabled by nanoscale solid electrolyte coating. Energy Storage Materials, 2020, 29, 71-77.	9.5	49
50	First-principles study of lattice dynamics of LiFePO4. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 4096-4100.	0.9	48
51	Structural, Electronic, and Li Migration Properties of RE-Doped (RE = Ce, La) LiCoO₂for Li-ion Batteries: A First-Principles Investigation. Journal of Physical Chemistry C, 2016, 120, 18428-18434.	1.5	48
52	Germagraphene as a promising anode material for lithium-ion batteries predicted from first-principles calculations. Nanoscale Horizons, 2019, 4, 457-463.	4.1	48
53	Three-dimensional honeycomb carbon: Junction line distortion and novel emergent fermions. Carbon, 2019, 141, 417-426.	5.4	48
54	Antisite defects and Mg doping in LiFePO4: aÂfirst-principles investigation. Applied Physics A: Materials Science and Processing, 2011, 104, 529-537.	1.1	47

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55	Lithium ion diffusion in Li4+xTi5O12: From ab initio studies. Electrochimica Acta, 2011, 56, 6084-6088.	2.6	46
56	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.	4.0	46
57	Mechanical properties of Wâ€“Ti alloys from first-principles calculations. Fusion Engineering and Design, 2016, 106, 34-39.	1.0	46
58	Bandgap tuning in MoSSe bilayers: synergistic effects of dipole moment and interlayer distance. Physical Chemistry Chemical Physics, 2018, 20, 20919-20926.	1.3	46
59	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.	0.9	45
60	Hydrogen-induced interactions in vanadium from first-principles calculations. Physical Review B, 2011, 83, .	1.1	45
61	Small polaron migration in LixMn2O4: From first principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2796-2799.	0.9	43
62	First-principles study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î³</mml:mi><mml:msub><mml:mrow><mml:mtext>-Al</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> surface. Physical Review B, 2009, 79, .	1.1	43
63	Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. National Science Review, 2020, 7, 1768-1775.	4.6	43
64	Crystal structure and electrochemical characteristics of non-AB5 type Laâ€“Ni system alloys. Journal of Power Sources, 2007, 164, 911-915.	4.0	41
65	Multiple Dirac Points and Hydrogenation-Induced Magnetism of Germanene Layer on Al (111) Surface. Journal of Physical Chemistry Letters, 2015, 6, 4936-4942.	2.1	41
66	Physics of electron and lithium-ion transport in electrode materials for Li-ion batteries. Chinese Physics B, 2016, 25, 018206.	0.7	41
67	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.	1.3	41
68	Insights into structural stability and Li superionic conductivity of Li10GeP2S12 from first-principles calculations. Chemical Physics Letters, 2014, 591, 16-20.	1.2	36
69	A first-principles investigation of Janus MoSSe as a catalyst for photocatalytic water-splitting. Applied Surface Science, 2021, 537, 147919.	3.1	36
70	Tuning the electronic properties of germanene by molecular adsorption and under an external electric field. Journal of Materials Chemistry C, 2018, 6, 5937-5948.	2.7	35
71	Coordination of lithium ion with ethylene carbonate electrolyte solvent: A computational study. International Journal of Quantum Chemistry, 2016, 116, 97-102.	1.0	33
72	Charge transfer and formation of Ce3+ upon adsorption of metal atom M (MÂ=ÂCu, Ag, Au) on CeO2 (100) surface. Journal of Power Sources, 2013, 234, 69-81.	4.0	32

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73	The structural and electronic properties of spinel MnCo2O4 bulk and low-index surfaces: From first principles studies. Applied Surface Science, 2015, 349, 510-515.	3.1	32
74	Lithium ion adsorption and diffusion on black phosphorene nanotube: A first-principles study. Applied Surface Science, 2017, 392, 88-94.	3.1	32
75	Is silicene stable in O ₂ ? â€"First-principles study of O ₂ dissociation and O ₂ -dissociationâ€"induced oxygen atoms adsorption on free-standing silicene. Europhysics Letters, 2014, 106, 47001.	0.7	31
76	Na2MnO3 as cathode materials for Na ion batteries: From first-principles investigations. Solid State Ionics, 2018, 320, 210-214.	1.3	31
77	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.	0.9	30
78	Ab initiostudies on the stability and electronic structure ofLiCoO2(003) surfaces. Physical Review B, 2005, 71, .	1.1	29
79	O-vacancy and surface on CeO2: A first-principles study. Journal of Physics and Chemistry of Solids, 2010, 71, 788-796.	1.9	29
80	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.	2.8	29
81	First-principles study of lithium intercalated bilayer graphene. Science China: Physics, Mechanics and Astronomy, 2012, 55, 1376-1382.	2.0	28
82	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.	0.7	28
83	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.	1.5	28
84	Understanding the effect of the layer-to-layer distance on Li-intercalated graphite. Journal of Applied Physics, 2012, 111, .	1.1	27
85	First-Principles Calculation of Lithium Adsorption and Diffusion on Silicene. Chinese Physics Letters, 2013, 30, 017103.	1.3	27
86	Jahnâ€"Teller type small polaron assisted Na diffusion in NaMnO₂as a cathode material for Na-ion batteries. Journal of Materials Chemistry A, 2019, 7, 6053-6061.	5.2	27
87	Role of alloying elements in vanadium-based binary alloy membranes for hydrogen separation. Journal of Membrane Science, 2012, 423-424, 332-341.	4.1	26
88	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.	2.0	25
89	Hydrogen storage on calcium-decorated BC7 sheet: A first-principles study. International Journal of Hydrogen Energy, 2014, 39, 2142-2148.	3.8	25
90	First Principles Study of Penta-siligraphene as High-Performance Anode Material for Li-Ion Batteries. Nanoscale Research Letters, 2019, 14, 260.	3.1	25

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91	The Role of Cu in Degrading Adsorption of CO on the Pt_nCu Clusters. Journal of Physical Chemistry A, 2013, 117, 8293-8297.	1.1	24
92	First principles study of g-Mg₃N₂ as an anode material for Na-, K-, Mg-, Ca- and Al-ion storage. RSC Advances, 2019, 9, 27378-27385.	1.7	24
93	Cobalt suppressed Jahnâ€“Teller effect in for lithium ion batteries. Solid State Communications, 2011, 151, 234-237.	0.9	23
94	STRAIN INDUCED ENHANCED MIGRATION OF POLARON AND LITHIUM ION IN Î»-MnO₂. Functional Materials Letters, 2012, 05, 1250037.	0.7	23
95	Ab initio investigation of Jahnâ€“Teller-distortion-tuned Li-ion migration in Î»-MnO₂. Journal of Materials Chemistry A, 2017, 5, 9618-9626.	5.2	23
96	Experimental and theoretical studies on dynamic properties of Li ions in LixMn2O4. Solid State Communications, 2004, 130, 501-506.	0.9	22
97	Pulsed laser deposition prepared LiMn 2 O 4 thin film. Thin Solid Films, 2006, 503, 268-271.	0.8	21
98	Density functional theory study of Ir atom deposited on Î³-Al2O3 (001) surface. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 277-281.	0.9	21
99	Transition from Mn4+ to Mn3+ induced by surface reconstruction at Î»-MnO2(001). Journal of Chemical Physics, 2010, 133, 204701.	1.2	21
100	The effect of strain on band structure of single-layer MoS2: an ab initio study. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 227102.	0.2	21
101	Polaron states and migration in F-doped Li2MnO3. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2449-2452.	0.9	20
102	First-principles study of the stability of free-standing germanene in oxygen atmosphere. Journal of Applied Physics, 2015, 118, 124303.	1.1	19
103	Organosilicon functionalized glycerol carbonates as electrolytes for lithium-ion batteries. RSC Advances, 2015, 5, 17660-17666.	1.7	19
104	Insights into the physics of interaction between borophene and O2-first-principles investigation. Computational Materials Science, 2017, 140, 261-266.	1.4	19
105	The adsorption and dissociation of oxygen on Ag (111) supported Ï‡ 3 borophene. Physica B: Condensed Matter, 2018, 537, 1-6.	1.3	18
106	First principles study of alkali and alkaline earth metal ions adsorption and diffusion on penta-graphene. Solid State Ionics, 2019, 342, 115062.	1.3	18
107	The effect of protons on the Mg²⁺ migration in an Î±-V₂O₅ cathode for magnesium batteries: a first-principles investigation. Physical Chemistry Chemical Physics, 2019, 21, 7406-7411.	1.3	18
108	First-principles study on electronic structure of LiFePO4. Solid State Communications, 2007, 143, 144-148.	0.9	17

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109	Li1+xFePO4 (0â‰¤xâ‰¤3) as anode material for lithium ion batteries: From ab initio studies. Journal of Power Sources, 2008, 175, 891-896.	4.0	17
110	Electronic structure and magnetism of EuX (X = O, S, Se and Te): A first-principles investigation. Europhysics Letters, 2008, 83, 69001.	0.7	17
111	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.	0.7	17
112	New insights into Li diffusion in Liâ€“Si alloys for Si anode materials: role of Si microstructures. Nanoscale, 2019, 11, 14042-14049.	2.8	17
113	First-Principles Study of Lithium and Sodium Atoms Intercalation in Fluorinated Graphite. Engineering, 2015, 1, 243-246.	3.2	16
114	The effect of titanium(Ti) doping on hydrogen incorporation in tungsten(W)ï¼šFirst-principles calculations. Fusion Engineering and Design, 2017, 121, 227-234.	1.0	16
115	Density functional theory prediction of Mg₃N₂ as a high-performance anode material for Li-ion batteries. Physical Chemistry Chemical Physics, 2019, 21, 7053-7060.	1.3	16
116	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.	0.7	16
117	Preparation and temperature-dependent photoluminescence properties of ScF₃:Eu³⁺submicroparticles. New Journal of Chemistry, 2017, 41, 7915-7923.	1.4	15
118	Calcium Doping of Lithium Titanium Oxide Nanospheres: A Combined Firstâ€Principles and Experimental Study. Energy Technology, 2017, 5, 539-543.	1.8	14
119	Confined Li ion migration in the silicon-graphene complex system: An ab initio investigation. Applied Surface Science, 2018, 436, 505-510.	3.1	14
120	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.	1.5	14
121	Iodine ion transport in solid electrolyte LiI(C3H5NO)2: a first-principles identification. Ionics, 2007, 12, 343-347.	1.2	13
122	Compressive strain induced dynamical stability of monolayer 1T-MX2 (Mâ€‰â€‰=â€‰â€‰Mo, W; Xâ€‰â€‰=â€‰â€‰S, Se). Ma Research Express, 2017, 4, 115018.	0.8	13
123	First-principles identification of spinel CaCo2O4 as a promising cathode material for Ca-ion batteries. Solid State Ionics, 2018, 326, 145-149.	1.3	13
124	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.	1.5	13
125	First-principles study on the electronic structures of Cr- and W-doped single-layer MoS2. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 037103.	0.2	13
126	Manipulation of spin-flip in Co3O4: a first principles study. Journal of Materials Science, 2016, 51, 4691-4696.	1.7	12

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127	Scandium Molybdate Microstructures with Tunable Phase and Morphology: Microwave Synthesis, Theoretical Calculations, and Photoluminescence Properties. Inorganic Chemistry, 2019, 58, 2491-2500.	1.9	12
128	First-principles study on the structural, electronic, and Li-ion mobility properties of anti-perovskite superionic conductor Li3OCl (1ÂÔÂ0) surface. Applied Surface Science, 2020, 510, 145394.	3.1	12
129	Hydrogen solution in tetrahedral or octahedral interstitial sites in Al. Journal of Alloys and Compounds, 2011, 509, 9214-9217.	2.8	11
130	Dissociation of (Li2O2)0,+ on graphene and boron-doped graphene: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2020, 22, 14216-14224.	1.3	11
131	Time dependence of the average charge and current in a dissipative mesoscopic circuit. Chinese Physics B, 2002, 11, 163-166.	1.3	10
132	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.	2.8	9
133	Interpenetrating graphene network bct-C₄₀: a promising anode material for Li ion batteries. Physical Chemistry Chemical Physics, 2019, 21, 23485-23491.	1.3	9
134	The structural, mechanical and electronic properties of (4,4) SiC/C nanotube heterojunction: A first-principles study. Computational Materials Science, 2013, 68, 367-370.	1.4	8
135	Further discussions on the geometry and fast diffusion of AlCl4 cluster intercalated in graphite. Electrochimica Acta, 2017, 223, 137-139.	2.6	8
136	Facile microwave synthesis of ScPO₄Â·2H₂O flowerlike superstructures: morphology control, electronic structure and multicolor tunable luminescent properties. CrystEngComm, 2017, 19, 5787-5796.	1.3	8
137	Shapiro effect in mesoscopic LC circuit. Chinese Physics B, 2002, 11, 720-724.	1.3	7
138	Electric-field-tunable molecular adsorption on germanane. Physical Chemistry Chemical Physics, 2019, 21, 20287-20295.	1.3	7
139	The effect of strain on the Li-storage performance of V2C and Nb2C: From first-principles study. Solid State Communications, 2020, 311, 113857.	0.9	7
140	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.	1.3	6
141	Comparative study on dynamical stability against strain of pristine and chemically functionalized monolayer honeycomb materials. Journal of Materials Science, 2018, 53, 4306-4315.	1.7	6
142	Electron-donor doping enhanced Li storage in electride Ca₂N monolayer: a first-principles study. Journal of Physics Condensed Matter, 2018, 30, 345501.	0.7	6
143	LiGaOS is a fast Li-Ion conductor: A first-principles prediction. Materials and Design, 2020, 185, 108264.	3.3	6
144	First-principles insights of hydrogen diffusion dynamics at the Î±-Al2O3 (0001) surface. Applied Surface Science, 2020, 531, 147263.	3.1	6

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145	First-principles study of Ï‡₃-borophene for charge-modulated switchable CO₂ capture. Physical Chemistry Chemical Physics, 2020, 22, 8864-8869.	1.3	6
146	Effects of Strain and Electric Field on Molecular Doping in MoSSe. ACS Omega, 2021, 6, 14639-14647.	1.6	6
147	First principles investigation of dynamic performance in the process of lithium intercalation into black phosphorus. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 247101.	0.2	6
148	The stability of free-standing germanane in oxygen: First-principles investigation. Europhysics Letters, 2015, 110, 17007.	0.7	5
149	Structural, electronic, sodium diffusion and elastic properties of Naâ€“P alloy anode for Na-ion batteries: Insight from first-principles calculations. Modern Physics Letters B, 2016, 30, 1650385.	1.0	5
150	The effect of titanium doping on carbon behavior in tungsten: A first-principles study. Fusion Engineering and Design, 2016, 112, 123-129.	1.0	5
151	Design and Properties Prediction of AMCO₃F by First-Principles Calculations. ACS Applied Materials & Interfaces, 2017, 9, 13255-13261.	4.0	5
152	Highly optimized embedding atom method potential for Pt-Cu alloys. Journal of Alloys and Compounds, 2017, 696, 470-480.	2.8	5
153	Curvature induced improvement of Li storage in Ca2N nanotubes. Applied Surface Science, 2018, 459, 406-410.	3.1	5
154	Structural and electronic properties of small lithium peroxide clusters in view of the charge process in Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2019, 21, 19935-19943.	1.3	5
155	The thermodynamics and electronic structure analysis of P-doped spinel Co3O4. Physical Chemistry Chemical Physics, 2021, 23, 3588-3594.	1.3	5
156	First-principles study on the electronic structures of Î²-SiC/carbon nanotube core-shell structures. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 107101.	0.2	5
157	Vacancy and H Interactions in Nb. Chinese Physics Letters, 2011, 28, 127101.	1.3	4
158	Effects of hydrogen on Mn-doped GaN: A first principles calculation. Physica B: Condensed Matter, 2013, 425, 38-41.	1.3	4
159	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.	1.3	4
160	The strain effect on lithium ion migration in Li-Si alloys: A first-principles study. Solid State Communications, 2016, 247, 47-52.	0.9	4
161	Structural and Electronic Features of Nb-Doped SrCoO₃: Insight from First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 24987-24993.	1.5	4
162	Strain-tunable molecular doping in germanane: a first-principles study. Nanotechnology, 2018, 29, 465202.	1.3	4

#	Article	IF	Citations
163	Strong Jahn-Teller effect at NiO4 tetrahedron in NiCo2O4 spinel. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126114.	0.9	4
164	Hydrogen solution in tungsten (W) under different temperatures and strains: a first principles calculation study. Physical Chemistry Chemical Physics, 2020, 22, 19623-19630.	1.3	4
165	Two-dimensional MnN utilized as high-capacity anode for Li-ion batteries*. Chinese Physics B, 2021, 30, 046302.	0.7	4
166	First-principles study of rare-earth-doped cathode materials Li₂MnO₃ in Li-ion batteries. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 138201.	0.2	4
167	STRAIN-TUNABLE BAND GAP OF BC₃ SHEET: A FIRST-PRINCIPLES INVESTIGATION. Modern Physics Letters B, 2013, 27, 1350110.	1.0	3
168	The Origin of BC ₇ Sheet Metallicity and the Tuning of its Electronic Properties by Hydrogenation. Chinese Physics Letters, 2013, 30, 066102.	1.3	3
169	First principle study of Li X S ₂ (X = Ga, In) as cathode materials for Li ion batteries. Chinese Physics B, 2016, 25, 028202.	0.7	3
170	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.	1.3	3
171	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.	5.2	3
172	First-principles calculation identification of ultrahigh hydrogen storage capacity in g-Mg3N2. Journal of Alloys and Compounds, 2021, 867, 158744.	2.8	3
173	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.	0.2	3
174	STRUCTURAL AND ELECTRONIC EVOLUTION FROM SiC SHEET TO SILICENE. International Journal of Modern Physics B, 2013, 27, 1350188.	1.0	2
175	Li ion diffusion dynamics on Li oxides and peroxides surfaces. Materials Letters, 2017, 188, 208-211.	1.3	2
176	Jahnâ€“Teller distortion affected Li ion migration in spinel TiO2. Solid State Ionics, 2017, 312, 17-20.	1.3	2
177	Adsorption of propylene carbonate on the LiMn₂O₄ (100) surface investigated by DFT + U calculations*. Chinese Physics B, 2021, 30, 038202.	0.7	2
178	First principles studies on the structural and electronic properties of Srn+1TinO3n+1 (n=1, 2, 3, âˆž). Physica B: Condensed Matter, 2010, 405, 4780-4784.	1.3	1
179	Curvature induced magnetic nanonodes in (6, 0) SiC/C nanotube heterojunction superlattice. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 58, 153-156.	1.3	1
180	Structural Features of Medium-Sized Ge n (nÂ=Â35, 40, 45, 50, 55 and 60) clusters. Journal of Cluster Science, 2015, 26, 1001-1010.	1.7	1

#	Article	IF	Citations
181	Vibrational and Thermodynamic Properties of Layered LiM0.5Ni0.5O2 (M=Mn, Co) Cathode Materials for Li Ion Batteries. International Journal of Electrochemical Science, 2017, , 2963-2972.	0.5	1
182	Molecular adsorption and strain-induced ferromagnetic semiconductor-metal transition in half-hydrogenated germanene. Journal of Applied Physics, 2019, 125, 082504.	1.1	1
183	Structural and Electronic Properties of Small Stoichiometric (Li2O2)n Clusters and Relevance to Liâ€“O2 Batteries. Journal of Cluster Science, 2020, 31, 643-649.	1.7	1
184	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.	0.8	1
185	Effect of strain on Li adsorption on silicene. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 217101.	0.2	1
186	FIRST-PRINCIPLES STUDY ON Î²-SiC/BNNT CORE/SHELL NANOCABLE. Modern Physics Letters B, 2013, 27, 1350169.	1.0	0
187	Ab initio molecular dynamics simulation of irradiation particles behavior in tungsten. European Physical Journal B, 2018, 91, 1.	0.6	0
188	An Sc-based coordination polymer with concaved superstructures: preparation, formation mechanism, conversion, and their electrochemistry properties. CrystEngComm, 2020, 22, 2926-2932.	1.3	0
189	Theoretical Studies on the Small Sized Lithium-silicon Clusters SinLi (n=1-10). Wuji Cailiao Xuebao/Journal of Inorganic Materials, 2013, 28, 1237-1242.	0.6	0