Xiaofeng Fan

List of Publications by Year
in descending order

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135 papers	8,103 citations	66234 42 h-index	51492 86 g-index
136 all docs	136 docs citations	136 times ranked	11991 citing authors

#	Article	IF	Citations
1	Mechanistic insights into the electrochemical Li/Na/K-ion storage for aqueous bismuth anode. Energy Storage Materials, 2022, 45, 33-39.	9.5	23
2	Favorable Energy Band Alignment of TiO₂ Anatase/Rutile Heterophase Homojunctions Yields Photocatalytic Hydrogen Evolution with Quantum Efficiency Exceeding 45.6%. Advanced Energy Materials, 2022, 12, .	10.2	106
3	Progress of graphdiyne-based materials for anodes of alkali metal ion batteries. Nano Futures, 2022, 6, 022004.	1.0	4
4	Favorable Energy Band Alignment of TiO₂ Anatase/Rutile Heterophase Homojunctions Yields Photocatalytic Hydrogen Evolution with Quantum Efficiency Exceeding 45.6% (Adv. Energy) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	10.2	0
5	Engineering of Transition Metal Sulfide Nanostructures as Efficient Electrodes for High-Performance Supercapacitors. ACS Applied Energy Materials, 2022, 5, 6481-6498.	2.5	68
6	Ultrafine Sb nanoparticles in situ confined in covalent organic frameworks for high-performance sodium-ion battery anodes. Journal of Materials Chemistry A, 2022, 10, 15089-15100.	5.2	19
7	Search for potential K ion battery cathodes by first principles. Journal of Energy Chemistry, 2021, 54, 377-385.	7.1	8
8	2D SnC sheet with a small strain is a promising Li host material for Li-ion batteries. Materials Today Communications, 2021, 26, 101768.	0.9	12
9	Storage mechanism of K in hydrogen-substituted graphdiyne as a superior anode. Journal of Materials Chemistry A, 2021, 9, 12320-12330.	5.2	4
10	Improved thermoelectric transport properties of Ge₄Se₃Te through dimensionality reduction. Journal of Materials Chemistry C, 2021, 9, 1804-1813.	2.7	17
11	Effect of voids on nanocrystalline gold ultrathin film. Computational Materials Science, 2021, 189, 110255.	1.4	4
12	Deformation and ductile fracture of nanocrystalline gold ultrathin nanoribbon: Width effect. Fatigue and Fracture of Engineering Materials and Structures, 2021, 44, 1850-1861.	1.7	5
13	Potential anodic applications of 2D MoS2 for K-ion batteries. Journal of Alloys and Compounds, 2021, 865, 158782.	2.8	38
14	Adsorption of K Ions on Single-Layer GeC for Potential Anode of K Ion Batteries. Nanomaterials, 2021, 11, 1900.	1.9	6
15	Interior Melting of Rapidly Heated Gold Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 8170-8177.	2.1	6
16	Lithiation and Sodiation of Hydrogenated Silicene: A Density Functional Theory Investigation. ChemSusChem, 2021, 14, 5460-5469.	3.6	14
17	First principles predictions of Na and K storage in layered SnSe2. Applied Surface Science, 2021, 566, 150522.	3.1	29
18	Shining light on chiral inorganic nanomaterials for biological issues. Theranostics, 2021, 11, 9262-9295.	4.6	27

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19	Strong Optical, Electrical, and Raman in-Plane Anisotropy in Corrugated Two-Dimensional Perovskite. Journal of Physical Chemistry C, 2021, 125, 22630-22642.	1.5	4
20	Reinventing the mechanism of high-performance Bi anode in aqueous K+ rechargeable batteries. Journal of Energy Chemistry, 2020, 48, 21-28.	7.1	34
21	Recent progress of TMD nanomaterials: phase transitions and applications. Nanoscale, 2020, 12, 1247-1268.	2.8	132
22	First principles and molecular dynamics study of Li wetting and diffusion on W surfaces. Journal of Nuclear Materials, 2020, 539, 152345.	1.3	8
23	The Effect of Strain Rate on the Deformation Processes of NC Gold with Small Grain Size. Crystals, 2020, 10, 858.	1.0	3
24	Adsorption and Diffusion of Potassium on 2D SnC Sheets for Potential Highâ€Performance Anodic Applications of Potassiumâ€Ion Batteries. ChemElectroChem, 2020, 7, 3832-3838.	1.7	33
25	First-Principles Calculation of Optimizing the Performance of Germanene-Based Supercapacitors by Vacancies and Metal Atoms. Journal of Physical Chemistry C, 2020, 124, 12346-12358.	1.5	16
26	Thermoelectric properties of monolayer GeAsSe and SnSbTe. Journal of Materials Chemistry C, 2020, 8, 9763-9774.	2.7	22
27	Heating-Rate and Particle-Size Effects on Melting Process of Au Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 7414-7420.	1.5	12
28	Copper-linked 1T MoS2/Cu2O Heterostructure for Efficient Photocatalytic Hydrogen Evolution. Chemical Research in Chinese Universities, 2020, 36, 1122-1127.	1.3	13
29	Nanocrystalline gold with small size: inverse Hallâ€“Petch between mixed regime and super-soft regime. Philosophical Magazine, 2020, 100, 2335-2351.	0.7	21
30	Ordered and disordered phases in WS_{2(1–}_{<italic>x</italic>}₎Se<sub>2</sub monolayer. Chinese Science Bulletin, 2020, 65, 856-864.		
31	The thermal and thermoelectric transport properties of SiSb, GeSb and SnSb monolayers. Journal of Materials Chemistry C, 2019, 7, 10652-10662.	2.7	36
32	Improving the Quantum Capacitance of Graphene-Based Supercapacitors by the Doping and Co-Doping: First-Principles Calculations. ACS Omega, 2019, 4, 13209-13217.	1.6	73
33	A Depth-Profiling Study on the Solid Electrolyte Interface: Bis(fluorosulfuryl)imide Anion toward Improved K⁺ Storage. ACS Applied Energy Materials, 2019, 2, 7942-7951.	2.5	51
34	Computational insight of monolayer SnS2 as anode material for potassium ion batteries. Applied Surface Science, 2019, 496, 143625.	3.1	63
35	Adsorption of metal atoms on silicene: stability and quantum capacitance of silicene-based electrode materials. Physical Chemistry Chemical Physics, 2019, 21, 4276-4285.	1.3	29
36	Staging: Unraveling the Potassium Storage Mechanism in Graphite Foam (Adv. Energy Mater. 22/2019). Advanced Energy Materials, 2019, 9, 1970081.	10.2	5

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37	Improving Polysulfides Adsorption and Redox Kinetics by the Co₄N Nanoparticle/Nâ€Doped Carbon Composites for Lithiumâ€Sulfur Batteries. Small, 2019, 15, e1901454.	5.2	130
38	Structural instability and magnetism of superconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KCr</mml:mi><mml:mn>3</mml:mn></mml Physical Review B, 2019, 99, .	1.3	11
39	Unraveling the Potassium Storage Mechanism in Graphite Foam. Advanced Energy Materials, 2019, 9, 1900579.	10.2	133
40	Lattice -Mismatch-Induced Ultrastable 1T-Phase MoS₂â€“Pd/Au for Plasmon-Enhanced Hydrogen Evolution. Nano Letters, 2019, 19, 2758-2764.	4.5	98
41	Layered Tl₂O: a model thermoelectric material. Journal of Materials Chemistry C, 2019, 7, 5094-5103.	2.7	46
42	Nitrogen configuration dependent holey active sites toward enhanced K+ storage in graphite foam. Journal of Power Sources, 2019, 419, 82-90.	4.0	36
43	Single-atom cobalt array bound to distorted 1T MoS2 with ensemble effect for hydrogen evolution catalysis. Nature Communications, 2019, 10, 5231.	5.8	371
44	Storage of Na in layered graphdiyne as high capacity anode materials for sodium ion batteries. Journal of Materials Chemistry A, 2019, 7, 25609-25618.	5.2	20
45	Nanopores in nanocrystalline gold. Materialia, 2019, 5, 100195.	1.3	8
46	Melting of Nanocrystalline Gold. Journal of Physical Chemistry C, 2019, 123, 907-914.	1.5	4
47	Iridium-Triggered Phase Transition of MoS₂ Nanosheets Boosts Overall Water Splitting in Alkaline Media. ACS Energy Letters, 2019, 4, 368-374.	8.8	105
48	Adsorption of Na on silicene for potential anode for Na-ion batteries. Electrochimica Acta, 2019, 297, 497-503.	2.6	35
49	Adsorption of Li on single-layer silicene for anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 8887-8896.	1.3	62
50	New design for highly durable infrared-reflective coatings. Light: Science and Applications, 2018, 7, 17175-17175.	7.7	37
51	DFT study on bimetallic Pt/Cu(1â€¯1â€¯1) as efficient catalyst for H2 dissociation. Applied Surface Science, 2018, 441, 23-28.	3.1	9
52	Quantum Capacitance of Silicene-Based Electrodes from First-Principles Calculations. Journal of Physical Chemistry C, 2018, 122, 1903-1912.	1.5	39
53	DFT calculation for stability and strength of iron borides. Computational Materials Science, 2018, 144, 147-153.	1.4	3
54	Oxidization of Al0.5Ga0.5As(001) surface: The electronic properties. Applied Surface Science, 2018, 436, 460-466.	3.1	7

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55	First principles study on 2Hâ€“1Tâ€² transition in MoS₂ with copper. Physical Chemistry Chemical Physics, 2018, 20, 26986-26994.	1.3	39
56	Modulation of Hydrogen Evolution Catalytic Activity of Basal Plane in Monolayer Platinum and Palladium Dichalcogenides. ACS Omega, 2018, 3, 10058-10065.	1.6	46
57	Thermoelectric properties of p-type cubic and rhombohedral GeTe. Journal of Applied Physics, 2018, 123, .	1.1	40
58	DFT Study on Intermetallic Pdâ€“Cu Alloy with Cover Layer Pd as Efficient Catalyst for Oxygen Reduction Reaction. Materials, 2018, 11, 33.	1.3	24
59	â€œElectron/Ion Spongeâ€•Like V-Based Polyoxometalate: Toward High-Performance Cathode for Rechargeable Sodium Ion Batteries. ACS Nano, 2017, 11, 6911-6920.	7.3	95
60	Adsorption and Formation of Small Na Clusters on Pristine and Double-Vacancy Graphene for Anodes of Na-Ion Batteries. ACS Applied Materials & Interfaces, 2017, 9, 17076-17084.	4.0	42
61	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. Journal of Applied Physics, 2017, 121, .	1.1	9
62	Hydrogen-Bonding Evolution during the Polymorphic Transformations in CH₃NH₃PbBr₃: Experiment and Theory. Chemistry of Materials, 2017, 29, 5974-5981.	3.2	80
63	Layer effect on catalytic activity of Pd-Cu bimetal for CO oxidation. Applied Catalysis A: General, 2017, 538, 66-73.	2.2	8
64	Vacuum level dependent photoluminescence in chemical vapor deposition-grown monolayer MoS 2. Scientific Reports, 2017, 7, 16714.	1.6	27
65	In Situ Observation and Electrochemical Study of Encapsulated Sulfur Nanoparticles by MoS₂ Flakes. Journal of the American Chemical Society, 2017, 139, 10133-10141.	6.6	126
66	Stability of Ptn cluster on free/defective graphene: A first-principles study. Applied Surface Science, 2017, 392, 936-941.	3.1	26
67	Ordered and Disordered Phases in Mo1â^'xWxS2 Monolayer. Scientific Reports, 2017, 7, 15124.	1.6	21
68	Electronic fitness function for screening semiconductors as thermoelectric materials. Physical Review Materials, 2017, 1, .	0.9	98
69	Modulation of electronic properties from stacking orders and spin-orbit coupling for 3R-type MoS2. Scientific Reports, 2016, 6, 24140.	1.6	23
70	Perspective: n-type oxide thermoelectrics via visual search strategies. APL Materials, 2016, 4, .	2.2	42
71	Pressure evolution of the potential barriers of phase transition of MoS₂, MoSe₂ and MoTe₂. Physical Chemistry Chemical Physics, 2016, 18, 12080-12085.	1.3	38
72	Valence Band Splitting on Multilayer MoS₂: Mixing of Spinâ€“Orbit Coupling and Interlayer Coupling. Journal of Physical Chemistry Letters, 2016, 7, 2175-2181.	2.1	73

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73	Oxidation of the titanium(0001) surface: diffusion processes of oxygen from DFT. RSC Advances, 2016, 6, 71311-71318.	1.7	21
74	Adsorption and diffusion of Li with S on pristine and defected graphene. Physical Chemistry Chemical Physics, 2016, 18, 31268-31276.	1.3	9
75	Array of nanosheets render ultrafast and high-capacity Na-ion storage by tunable pseudocapacitance. Nature Communications, 2016, 7, 12122.	5.8	1,232
76	Controlling phase transition for single-layer MTe₂ (M = Mo and W): modulation of the potential barrier under strain. Physical Chemistry Chemical Physics, 2016, 18, 4086-4094.	1.3	105
77	Transparent conductivity modulation of ZnO by group-IVA doping. Chemical Physics Letters, 2016, 649, 78-83.	1.2	3
78	Density functional theory study of Li binding to graphene. RSC Advances, 2016, 6, 26540-26545.	1.7	21
79	Probing Spinâ€“Orbit Coupling and Interlayer Coupling in Atomically Thin Molybdenum Disulfide Using Hydrostatic Pressure. ACS Nano, 2016, 10, 1619-1624.	7.3	47
80	Magnetism in Na-filled Fe-based skutterudites. Scientific Reports, 2015, 5, 10782.	1.6	12
81	Transparent conducting properties of SrSnO₃ and ZnSnO₃. APL Materials, 2015, 3, 062505.	2.2	65
82	Structural stability of single-layer MoS₂ under large strain. Journal of Physics Condensed Matter, 2015, 27, 105401.	0.7	29
83	Transformation of electronic properties and structural phase transition from HfN to Hf₃N₄. Journal of Physics Condensed Matter, 2015, 27, 225501.	0.7	7
84	Identification of a potential superhard compound ReCN. Journal of Alloys and Compounds, 2015, 631, 321-327.	2.8	9
85	Identification and thermodynamic mechanism of the phase transition in hafnium nitride films. Acta Materialia, 2015, 90, 59-68.	3.8	31
86	Negative effect of vacancies on cubic symmetry, hardness and conductivity in hafnium nitride films. Scripta Materialia, 2015, 108, 141-146.	2.6	25
87	Density Functional Theory Calculations for the Quantum Capacitance Performance of Graphene-Based Electrode Material. Journal of Physical Chemistry C, 2015, 119, 6464-6470.	1.5	166
88	The Electronic Properties of Single-Layer and Multilayer MoS₂ under High Pressure. Journal of Physical Chemistry C, 2015, 119, 10189-10196.	1.5	89
89	Pressure evolution of the potential barriers for transformations of layered BN to dense structures. RSC Advances, 2015, 5, 87550-87555.	1.7	3
90	2DEGs at Perovskite Interfaces between KTaO3 or KNbO3 and Stannates. PLoS ONE, 2014, 9, e91423.	1.1	32

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91	Strain dependence of the optical properties and band gap of transparent conducting BaSnO₃and SrSnO₃. Proceedings of SPIE, 2014, , .	0.8	0
92	Nature of Tunable Optical Reflectivity of Rocksalt Hafnium Nitride Films. Journal of Physical Chemistry C, 2014, 118, 20511-20520.	1.5	23
93	On the nature of point defect and its effect on electronic structure of rocksalt hafnium nitride films. Acta Materialia, 2014, 81, 315-325.	3.8	31
94	Shape-dependent catalytic activity of oxygen reduction reaction (ORR) on silver nanodecahedra and nanocubes. Journal of Power Sources, 2014, 269, 152-157.	4.0	89
95	Light scattering and surface plasmons on small spherical particles. Light: Science and Applications, 2014, 3, e179-e179.	7.7	450
96	Adsorption of Single Li and the Formation of Small Li Clusters on Graphene for the Anode of Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2013, 5, 7793-7797.	4.0	190
97	Electrical and Photoresponse Properties of Printed Thin-Film Transistors Based on Poly(9,9-dioctylfluorene-co-bithiophene) Sorted Large-Diameter Semiconducting Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 18243-18250.	1.5	76
98	First-principles study on the structure, elastic properties, hardness and electronic structure of TMB4 (TM=Cr, Re, Ru and Os) compounds. Journal of Solid State Chemistry, 2013, 207, 29-34.	1.4	34
99	First-principle calculations on the structural stability and electronic properties of superhard B_xC_ycompounds. Journal of Physics Condensed Matter, 2013, 25, 045502.	0.7	8
100	Orbital analysis of electronic structure and phonon dispersion in MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, MoSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, WS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	343
101	Oxygen reduction reaction on active sites of heteroatom-doped graphene. RSC Advances, 2013, 3, 5498.	1.7	59
102	Relationship between dielectric coefficient and Urbach tail width of hydrogenated amorphous germanium carbon alloy films. Applied Physics Letters, 2012, 101, 042109.	1.5	10
103	Interaction between graphene and the surface of SiO₂. Journal of Physics Condensed Matter, 2012, 24, 305004.	0.7	69
104	Band Gap Tuning of Graphene by Adsorption of Aromatic Molecules. Journal of Physical Chemistry C, 2012, 116, 13788-13794.	1.5	85
105	Band gap opening of graphene by doping small boron nitride domains. Nanoscale, 2012, 4, 2157.	2.8	225
106	Metal free hydrogenation reaction on carbon doped boron nitride fullerene: A DFT study on the kinetic issue. International Journal of Hydrogen Energy, 2012, 37, 14336-14342.	3.8	94
107	Adsorption and Diffusion of Li on Pristine and Defective Graphene. ACS Applied Materials & Interfaces, 2012, 4, 2432-2438.	4.0	363
108	DFT Study of Hydrogen Storage by Spillover on Graphene with Boron Substitution. Journal of Physical Chemistry C, 2011, 115, 9241-9249.	1.5	129

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109	Memetic figure selection for cluster expansion in binary alloy systems. , 2011, , .		0
110	FeCl₃â€Based Fewâ€Layer Graphene Intercalation Compounds: Single Linear Dispersion Electronic Band Structure and Strong Charge Transfer Doping. Advanced Functional Materials, 2010, 20, 3504-3509.	7.8	154
111	Enrichment of (8,4) Singleâ€Walled Carbon Nanotubes Through Coextraction with Heparin. Small, 2010, 6, 110-118.	5.2	27
112	Direct enumeration of wurtzite BC2N configurations for structural stability and hardness evaluation. Diamond and Related Materials, 2010, 19, 100-105.	1.8	4
113	Carbon doped boron nitride cages as competitive candidates for hydrogen storage materials. Chemical Communications, 2010, 46, 883-885.	2.2	42
114	The role of sp-hybridized atoms in carbon ferromagnetism: a spin-polarized density functional theory calculation. Journal of Physics Condensed Matter, 2010, 22, 046001.	0.7	5
115	Huge light scattering from active anisotropic spherical particles. Optics Express, 2010, 18, 24868.	1.7	22
116	Composition-temperature phase diagram of BexZn1â^'xO from first principles. Computational Materials Science, 2010, 49, S29-S31.	1.4	25
117	Predicting the hydrogen bond ordered structures of ice Ih, II, III, VI and ice VII: DFT methods with localized based set. Computational Materials Science, 2010, 49, S170-S175.	1.4	28
118	Functionalizing Single- and Multi-layer Graphene with Br and Br2. Journal of Physical Chemistry C, 2010, 114, 14939-14945.	1.5	43
119	Local structure relaxation, quantum trap depression, and valence charge polarization induced by the shorter-and-stronger bonds between under-coordinated atoms in gold nanostructures. Nanoscale, 2010, 2, 412-417.	2.8	36
120	Ultrafast carrier dynamics in pristine and FeCl3-intercalated bilayer graphene. Applied Physics Letters, 2010, 97, 141910.	1.5	28
121	The valence charge polarization induced by the shorter and stronger bonds between under-coordinated gold atoms. , 2010, , .		0
122	Theoretical Study on Structural Stability of Alloy Cages: a Case of Silicon-doped Heterofullerenes. Communications in Computational Physics, 2010, 8, 289-303.	0.7	4
123	Roles of Cu codoping and oxygen vacancies on ferromagnetism in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2009, 79, .	1.1	31
124	First-principles study of the magnetization of oxygen-depleted In₂O₃(001) surfaces. Journal of Physics Condensed Matter, 2009, 21, 272202.	0.7	22
125	Energy Transfer from Photo-Excited Fluorene Polymers to Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 14946-14952.	1.5	54
126	A theoretical study of thermal stability and electronic properties of wurtzite and zincblende ZnO_xS_{1â^'x}. New Journal of Physics, 2009, 11, 093008.	1.2	42

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127	A first-principle study on the structure, stability and hardness of cubic BC2N. Diamond and Related Materials, 2009, 18, 1278-1282.	1.8	21
128	Density Functional Theory Study of Finite Carbon Chains. ACS Nano, 2009, 3, 3788-3794.	7.3	56
129	Theoretical Study of the Structural and Electronic Properties of SimGen and SimGen- (s = m + n â‰¤ 7) Clusters. Journal of Physical Chemistry A, 2008, 112, 2235-2241.	1.1	13
130	Orientation-Dependent Raman Spectroscopy of Single Wurtzite CdS Nanowires. Journal of Physical Chemistry C, 2008, 112, 1865-1870.	1.5	83
131	A first-principle analysis on the phase stabilities, chemical bonds and band gaps of wurtzite structure A_xZn_{1â^'x}O alloys (A = Ca, Cd, Mg). Journal of Physics Condensed Matter, 2008, 20, 235221.	0.7	67
132	On the Use of Bond-Counting Rules in Predicting the Stability of C₁₂B₆N₆ Fullerene. Journal of Physical Chemistry C, 2008, 112, 15691-15696.	1.5	24
133	Visualization and investigation of Siâ€“C covalent bonding of single carbon nanotube grown on silicon substrate. Applied Physics Letters, 2008, 93, 103111.	1.5	14
134	Anisotropy of electron-phonon coupling in single wurtzite CdS nanowires. Applied Physics Letters, 2007, 91, .	1.5	41
135	A direct first principles study on the structure and electronic properties of BexZn1â^'xO. Applied Physics Letters, 2007, 91, 121121.	1.5	64