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	Array of nanosheets render ultrafast and high-capacity Na-ion storage by tunable pseudocapacitance. Nature Communications, 2016, 7, 12122.	5.8	1,232
2	Light scattering and surface plasmons on small spherical particles. Light: Science and Applications, 2014, 3, e179-e179.	7.7	450
3	Single-atom cobalt array bound to distorted 1T MoS2 with ensemble effect for hydrogen evolution catalysis. Nature Communications, 2019, 10, 5231.	5.8	371
4	Adsorption and Diffusion of Li on Pristine and Defective Graphene. ACS Applied Materials & Interfaces, 2012, 4, 2432-2438.	4.0	363
5	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:mml:	1.1	343
6	Band gap opening of graphene by doping small boron nitride domains. Nanoscale, 2012, 4, 2157.	2.8	225
7	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
8	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
9	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
10	Unraveling the Potassium Storage Mechanism in Graphite Foam. Advanced Energy Materials, 2019, 9, 1900579.	10.2	133
11	Recent progress of TMD nanomaterials: phase transitions and applications. Nanoscale, 2020, 12, 1247-1268.	2.8	132
12	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
13	DFT Study of Hydrogen Storage by Spillover on Graphene with Boron Substitution. Journal of Physical Chemistry C, 2011, 115, 9241-9249.	1.5	129
14	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
15	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
16	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
17	Iridium-Triggered Phase Transition of MoS₂ Nanosheets Boosts Overall Water Splitting in Alkaline Media. ACS Energy Letters, 2019, 4, 368-374.	8.8	105
18	Lattice -Mismatch-Induced Ultrastable 1T-Phase MoS₂â€“Pd/Au for Plasmon-Enhanced Hydrogen Evolution. Nano Letters, 2019, 19, 2758-2764.	4.5	98

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19	Electronic fitness function for screening semiconductors as thermoelectric materials. Physical Review Materials, 2017, 1, .	0.9	98
20	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
21	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
22	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
23	The Electronic Properties of Single-Layer and Multilayer MoS₂ under High Pressure. Journal of Physical Chemistry C, 2015, 119, 10189-10196.	1.5	89
24	Band Gap Tuning of Graphene by Adsorption of Aromatic Molecules. Journal of Physical Chemistry C, 2012, 116, 13788-13794.	1.5	85
25	Orientation-Dependent Raman Spectroscopy of Single Wurtzite CdS Nanowires. Journal of Physical Chemistry C, 2008, 112, 1865-1870.	1.5	83
26	Hydrogen-Bonding Evolution during the Polymorphic Transformations in CH₃NH₃PbBr₃: Experiment and Theory. Chemistry of Materials, 2017, 29, 5974-5981.	3.2	80
27	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
28	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
29	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
30	Interaction between graphene and the surface of SiO₂. Journal of Physics Condensed Matter, 2012, 24, 305004.	0.7	69
31	Engineering of Transition Metal Sulfide Nanostructures as Efficient Electrodes for High-Performance Supercapacitors. ACS Applied Energy Materials, 2022, 5, 6481-6498.	2.5	68
32	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
33	Transparent conducting properties of SrSnO₃ and ZnSnO₃. APL Materials, 2015, 3, 062505.	2.2	65
34	A direct first principles study on the structure and electronic properties of BexZn1â^'xO. Applied Physics Letters, 2007, 91, 121121.	1.5	64
35	Computational insight of monolayer SnS2 as anode material for potassium ion batteries. Applied Surface Science, 2019, 496, 143625.	3.1	63
36	Adsorption of Li on single-layer silicene for anodes of Li-ion batteries. Physical Chemistry Chemical Physics, 2018, 20, 8887-8896.	1.3	62

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37	Oxygen reduction reaction on active sites of heteroatom-doped graphene. RSC Advances, 2013, 3, 5498.	1.7	59
38	Density Functional Theory Study of Finite Carbon Chains. ACS Nano, 2009, 3, 3788-3794.	7.3	56
39	Energy Transfer from Photo-Excited Fluorene Polymers to Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 14946-14952.	1.5	54
40	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
41	Probing Spinâ€“Orbit Coupling and Interlayer Coupling in Atomically Thin Molybdenum Disulfide Using Hydrostatic Pressure. ACS Nano, 2016, 10, 1619-1624.	7.3	47
42	Modulation of Hydrogen Evolution Catalytic Activity of Basal Plane in Monolayer Platinum and Palladium Dichalcogenides. ACS Omega, 2018, 3, 10058-10065.	1.6	46
43	Layered Tl₂O: a model thermoelectric material. Journal of Materials Chemistry C, 2019, 7, 5094-5103.	2.7	46
44	Functionalizing Single- and Multi-layer Graphene with Br and Br2. Journal of Physical Chemistry C, 2010, 114, 14939-14945.	1.5	43
45	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
46	Carbon doped boron nitride cages as competitive candidates for hydrogen storage materials. Chemical Communications, 2010, 46, 883-885.	2.2	42
47	Perspective: n-type oxide thermoelectrics via visual search strategies. APL Materials, 2016, 4, .	2.2	42
48	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
49	Anisotropy of electron-phonon coupling in single wurtzite CdS nanowires. Applied Physics Letters, 2007, 91, .	1.5	41
50	Thermoelectric properties of p-type cubic and rhombohedral GeTe. Journal of Applied Physics, 2018, 123, .	1.1	40
51	Quantum Capacitance of Silicene-Based Electrodes from First-Principles Calculations. Journal of Physical Chemistry C, 2018, 122, 1903-1912.	1.5	39
52	First principles study on 2Hâ€“1Tâ€² transition in MoS₂ with copper. Physical Chemistry Chemical Physics, 2018, 20, 26986-26994.	1.3	39
53	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
54	Potential anodic applications of 2D MoS2 for K-ion batteries. Journal of Alloys and Compounds, 2021, 865, 158782.	2.8	38

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55	New design for highly durable infrared-reflective coatings. Light: Science and Applications, 2018, 7, 17175-17175.	7.7	37
56	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
57	The thermal and thermoelectric transport properties of SiSb, GeSb and SnSb monolayers. Journal of Materials Chemistry C, 2019, 7, 10652-10662.	2.7	36
58	Nitrogen configuration dependent holey active sites toward enhanced K+ storage in graphite foam. Journal of Power Sources, 2019, 419, 82-90.	4.0	36
59	Adsorption of Na on silicene for potential anode for Na-ion batteries. Electrochimica Acta, 2019, 297, 497-503.	2.6	35
60	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
61	Reinventing the mechanism of high-performance Bi anode in aqueous K+ rechargeable batteries. Journal of Energy Chemistry, 2020, 48, 21-28.	7.1	34
62	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
63	2DEGs at Perovskite Interfaces between KTaO3 or KNbO3 and Stannates. PLoS ONE, 2014, 9, e91423.	1.1	32
64	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:msub> Physical Review B, 2009, 79, .	1.1	31
65	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
66	Identification and thermodynamic mechanism of the phase transition in hafnium nitride films. Acta Materialia, 2015, 90, 59-68.	3.8	31
67	Structural stability of single-layer MoS₂ under large strain. Journal of Physics Condensed Matter, 2015, 27, 105401.	0.7	29
68	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
69	First principles predictions of Na and K storage in layered SnSe2. Applied Surface Science, 2021, 566, 150522.	3.1	29
70	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
71	Ultrafast carrier dynamics in pristine and FeCl3-intercalated bilayer graphene. Applied Physics Letters, 2010, 97, 141910.	1.5	28
72	Enrichment of (8,4) Singleâ€Walled Carbon Nanotubes Through Coextraction with Heparin. Small, 2010, 6, 110-118.	5.2	27

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73	Vacuum level dependent photoluminescence in chemical vapor deposition-grown monolayer MoS 2. Scientific Reports, 2017, 7, 16714.	1.6	27
74	Shining light on chiral inorganic nanomaterials for biological issues. Theranostics, 2021, 11, 9262-9295.	4.6	27
75	Stability of Ptn cluster on free/defective graphene: A first-principles study. Applied Surface Science, 2017, 392, 936-941.	3.1	26
76	Composition-temperature phase diagram of BexZn1â^'xO from first principles. Computational Materials Science, 2010, 49, S29-S31.	1.4	25
77	Negative effect of vacancies on cubic symmetry, hardness and conductivity in hafnium nitride films. Scripta Materialia, 2015, 108, 141-146.	2.6	25
78	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
79	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
80	Nature of Tunable Optical Reflectivity of Rocksalt Hafnium Nitride Films. Journal of Physical Chemistry C, 2014, 118, 20511-20520.	1.5	23
81	Modulation of electronic properties from stacking orders and spin-orbit coupling for 3R-type MoS2. Scientific Reports, 2016, 6, 24140.	1.6	23
82	Mechanistic insights into the electrochemical Li/Na/K-ion storage for aqueous bismuth anode. Energy Storage Materials, 2022, 45, 33-39.	9.5	23
83	First-principles study of the magnetization of oxygen-depleted In₂O₃(001) surfaces. Journal of Physics Condensed Matter, 2009, 21, 272202.	0.7	22
84	Huge light scattering from active anisotropic spherical particles. Optics Express, 2010, 18, 24868.	1.7	22
85	Thermoelectric properties of monolayer GeAsSe and SnSbTe. Journal of Materials Chemistry C, 2020, 8, 9763-9774.	2.7	22
86	A first-principle study on the structure, stability and hardness of cubic BC2N. Diamond and Related Materials, 2009, 18, 1278-1282.	1.8	21
87	Oxidation of the titanium(0001) surface: diffusion processes of oxygen from DFT. RSC Advances, 2016, 6, 71311-71318.	1.7	21
88	Density functional theory study of Li binding to graphene. RSC Advances, 2016, 6, 26540-26545.	1.7	21
89	Ordered and Disordered Phases in Mo1â^'xWxS2 Monolayer. Scientific Reports, 2017, 7, 15124.	1.6	21
90	Nanocrystalline gold with small size: inverse Hallâ€“Petch between mixed regime and super-soft regime. Philosophical Magazine, 2020, 100, 2335-2351.	0.7	21

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91	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
92	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
93	Improved thermoelectric transport properties of Ge₄Se₃Te through dimensionality reduction. Journal of Materials Chemistry C, 2021, 9, 1804-1813.	2.7	17
94	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
95	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
96	Lithiation and Sodiation of Hydrogenated Silicene: A Density Functional Theory Investigation. ChemSusChem, 2021, 14, 5460-5469.	3.6	14
97	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
98	Copper-linked 1T MoS2/Cu2O Heterostructure for Efficient Photocatalytic Hydrogen Evolution. Chemical Research in Chinese Universities, 2020, 36, 1122-1127.	1.3	13
99	Magnetism in Na-filled Fe-based skutterudites. Scientific Reports, 2015, 5, 10782.	1.6	12
100	Heating-Rate and Particle-Size Effects on Melting Process of Au Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 7414-7420.	1.5	12
101	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
102	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	1.3	11
	Physical Review B, 2019, 99, .		
103	Relationship between dielectric coefficient and Urbach tail width of hydrogenated amorphous germanium carbon alloy films. Applied Physics Letters, 2012, 101, 042109.	1.5	10
104	Identification of a potential superhard compound ReCN. Journal of Alloys and Compounds, 2015, 631, 321-327.	2.8	9
105	Adsorption and diffusion of Li with S on pristine and defected graphene. Physical Chemistry Chemical Physics, 2016, 18, 31268-31276.	1.3	9
106	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. Journal of Applied Physics, 2017, 121, .	1.1	9
107	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
108	First-principle calculations on the structural stability and electronic properties of superhard B_xC_ycompounds. Journal of Physics Condensed Matter, 2013, 25, 425502.	0.7	8

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109	Layer effect on catalytic activity of Pd-Cu bimetal for CO oxidation. Applied Catalysis A: General, 2017, 538, 66-73.	2.2	8
110	Nanopores in nanocrystalline gold. Materialia, 2019, 5, 100195.	1.3	8
111	First principles and molecular dynamics study of Li wetting and diffusion on W surfaces. Journal of Nuclear Materials, 2020, 539, 152345.	1.3	8
112	Search for potential K ion battery cathodes by first principles. Journal of Energy Chemistry, 2021, 54, 377-385.	7.1	8
113	Transformation of electronic properties and structural phase transition from HfN to Hf₃N₄. Journal of Physics Condensed Matter, 2015, 27, 225501.	0.7	7
114	Oxidization of Al0.5Ga0.5As(001) surface: The electronic properties. Applied Surface Science, 2018, 436, 460-466.	3.1	7
115	Adsorption of K Ions on Single-Layer GeC for Potential Anode of K Ion Batteries. Nanomaterials, 2021, 11, 1900.	1.9	6
116	Interior Melting of Rapidly Heated Gold Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 8170-8177.	2.1	6
117	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
118	Staging: Unraveling the Potassium Storage Mechanism in Graphite Foam (Adv. Energy Mater. 22/2019). Advanced Energy Materials, 2019, 9, 1970081.	10.2	5
119	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
120	Direct enumeration of wurtzite BC2N configurations for structural stability and hardness evaluation. Diamond and Related Materials, 2010, 19, 100-105.	1.8	4
121	Melting of Nanocrystalline Gold. Journal of Physical Chemistry C, 2019, 123, 907-914.	1.5	4
122	Storage mechanism of K in hydrogen-substituted graphdiyne as a superior anode. Journal of Materials Chemistry A, 2021, 9, 12320-12330.	5.2	4
123	Effect of voids on nanocrystalline gold ultrathin film. Computational Materials Science, 2021, 189, 110255.	1.4	4
124	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
125	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
126	Progress of graphdiyne-based materials for anodes of alkali metal ion batteries. Nano Futures, 2022, 6, 022004.	1.0	4

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127	Pressure evolution of the potential barriers for transformations of layered BN to dense structures. RSC Advances, 2015, 5, 87550-87555.	1.7	3
128	Transparent conductivity modulation of ZnO by group-IVA doping. Chemical Physics Letters, 2016, 649, 78-83.	1.2	3
129	DFT calculation for stability and strength of iron borides. Computational Materials Science, 2018, 144, 147-153.	1.4	3
130	The Effect of Strain Rate on the Deformation Processes of NC Gold with Small Grain Size. Crystals, 2020, 10, 858.	1.0	3
131	The valence charge polarization induced by the shorter and stronger bonds between under-coordinated gold atoms. , 2010, , .		0
132	Memetic figure selection for cluster expansion in binary alloy systems. , 2011, , .		0
133	Strain dependence of the optical properties and band gap of transparent conducting BaSnO₃and SrSnO₃. Proceedings of SPIE, 2014, , .	0.8	0
134	Ordered and disordered phases in WS_{2(1–}_{<italic>x</italic>}₎Se<sub>2</sub monolayer. Chinese Science Bulletin, 2020, 65, 856-864.		
135	Favorable Energy Band Alignment of TiO₂ Anatase/Rutile Heterophase Homojunctions Yields Photocatalytic Hydrogen Evolution with Quantum Efficiency Exceeding 45.6% (Adv. Energy) Tj ETQq1 1 0.784314 rgBT /Overlock	10.1	