Aijun Du

List of Publications by Year in descending order

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Version: 2024-02-01

347 papers	29,944 citations	5891 81 h-index	5820 161 g-index
356 all docs	356 docs citations	356 times ranked	27426 citing authors

#	Article	IF	Citations
1	Hydrogen evolution by a metal-free electrocatalyst. Nature Communications, 2014, 5, 3783.	5.8	1,851
2	Ti3C2 MXene co-catalyst on metal sulfide photo-absorbers for enhanced visible-light photocatalytic hydrogen production. Nature Communications, 2017, 8, 13907.	5.8	1,496
3	Single Atom (Pd/Pt) Supported on Graphitic Carbon Nitride as an Efficient Photocatalyst for Visible-Light Reduction of Carbon Dioxide. Journal of the American Chemical Society, 2016, 138, 6292-6297.	6.6	985
4	Defect Graphene as a Trifunctional Catalyst for Electrochemical Reactions. Advanced Materials, 2016, 28, 9532-9538.	11.1	961
5	Nanoporous Graphitic-C₃N₄@Carbon Metal-Free Electrocatalysts for Highly Efficient Oxygen Reduction. Journal of the American Chemical Society, 2011, 133, 20116-20119.	6.6	958
6	A Heterostructure Coupling of Exfoliated Niâ€“Fe Hydroxide Nanosheet and Defective Graphene as a Bifunctional Electrocatalyst for Overall Water Splitting. Advanced Materials, 2017, 29, 1700017.	11.1	845
7	2D MXenes: A New Family of Promising Catalysts for the Hydrogen Evolution Reaction. ACS Catalysis, 2017, 7, 494-500.	5.5	825
8	Metal-Free Single Atom Catalyst for N₂ Fixation Driven by Visible Light. Journal of the American Chemical Society, 2018, 140, 14161-14168.	6.6	742
9	Graphene Defects Trap Atomic Ni Species for Hydrogen and Oxygen Evolution Reactions. CheM, 2018, 4, 285-297.	5.8	624
10	Hybrid Graphene and Graphitic Carbon Nitride Nanocomposite: Gap Opening, Electronâ€“Hole Puddle, Interfacial Charge Transfer, and Enhanced Visible Light Response. Journal of the American Chemical Society, 2012, 134, 4393-4397.	6.6	565
11	Understanding the Enhancement in Photoelectrochemical Properties of Photocatalytically Prepared TiO₂-Reduced Graphene Oxide Composite. Journal of Physical Chemistry C, 2011, 115, 6004-6009.	1.5	403
12	Organicâ€“inorganic bismuth (III)-based material: A lead-free, air-stable and solution-processable light-absorber beyond organolead perovskites. Nano Research, 2016, 9, 692-702.	5.8	351
13	Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. Chemical Communications, 2011, 47, 11843.	2.2	329
14	Towards lead-free perovskite photovoltaics and optoelectronics by ab-initio simulations. Scientific Reports, 2017, 7, 14025.	1.6	310
15	Multifunctional Porous Graphene for Nanoelectronics and Hydrogen Storage: New Properties Revealed by First Principle Calculations. Journal of the American Chemical Society, 2010, 132, 2876-2877.	6.6	304
16	A General Twoâ€Step Strategyâ€“Based Highâ€Throughput Screening of Single Atom Catalysts for Nitrogen Fixation. Small Methods, 2019, 3, 1800376.	4.6	303
17	Charge Mediated Semiconducting-to-Metallic Phase Transition in Molybdenum Disulfide Monolayer and Hydrogen Evolution Reaction in New 1Tâ€² Phase. Journal of Physical Chemistry C, 2015, 119, 13124-13128.	1.5	295
18	Charge-Controlled Switchable CO₂ Capture on Boron Nitride Nanomaterials. Journal of the American Chemical Society, 2013, 135, 8246-8253.	6.6	293

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19	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. Nano Letters, 2019, 19, 1366-1370.	4.5	292
20	First-Principles Prediction of Metal-Free Magnetism and Intrinsic Half-Metallicity in Graphitic Carbon Nitride. Physical Review Letters, 2012, 108, 197207.	2.9	272
21	Understanding the Roles of Oxygen Vacancies in Hematiteâ€Based Photoelectrochemical Processes. Angewandte Chemie - International Edition, 2019, 58, 1030-1034.	7.2	268
22	Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole Doping, and Sensitization for Visible Light Response. Journal of Physical Chemistry Letters, 2011, 2, 894-899.	2.1	252
23	New Ironâ€Cobalt Oxide Catalysts Promoting BiVO₄ Films for Photoelectrochemical Water Splitting. Advanced Functional Materials, 2018, 28, 1802685.	7.8	248
24	Synergistic crystal facet engineering and structural control of WO3 films exhibiting unprecedented photoelectrochemical performance. Nano Energy, 2016, 24, 94-102.	8.2	243
25	In Situ Formation of Oxygen Vacancies Achieving Nearâ€Complete Charge Separation in Planar BiVO₄ Photoanodes. Advanced Materials, 2020, 32, e2001385.	11.1	236
26	Single Molybdenum Atom Anchored on N-Doped Carbon as a Promising Electrocatalyst for Nitrogen Reduction into Ammonia at Ambient Conditions. Journal of Physical Chemistry C, 2018, 122, 16842-16847.	1.5	223
27	Graphene-like Two-Dimensional Ionic Boron with Double Dirac Cones at Ambient Condition. Nano Letters, 2016, 16, 3022-3028.	4.5	222
28	Moltenâ€Saltâ€Mediated Synthesis of an Atomic Nickel Coâ€catalyst on TiO₂ for Improved Photocatalytic H₂ Evolution. Angewandte Chemie - International Edition, 2020, 59, 7230-7234.	7.2	221
29	Edgeâ€Rich Feâ€'N₄ Active Sites in Defective Carbon for Oxygen Reduction Catalysis. Advanced Materials, 2020, 32, e2000966.	11.1	215
30	An Intrinsically Nonâ€flammable Electrolyte for Highâ€Performance Potassium Batteries. Angewandte Chemie - International Edition, 2020, 59, 3638-3644.	7.2	211
31	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. Journal of Physical Chemistry C, 2015, 119, 6918-6922.	1.5	210
32	Dirac State in the FeB₂ Monolayer with Graphene-Like Boron Sheet. Nano Letters, 2016, 16, 6124-6129.	4.5	200
33	Anti-fouling graphene-based membranes for effective water desalination. Nature Communications, 2018, 9, 683.	5.8	197
34	Transitionâ€Metal Single Atoms Anchored on Graphdiyne as Highâ€Efficiency Electrocatalysts for Water Splitting and Oxygen Reduction. Small Methods, 2019, 3, 1800419.	4.6	192
35	Rapid microwave-assisted synthesis of Mn3O4â€“graphene nanocomposite and its lithium storage properties. Journal of Materials Chemistry, 2012, 22, 3600.	6.7	183
36	First-principle studies of electronic structure and C-doping effect in boron nitride nanoribbon. Chemical Physics Letters, 2007, 447, 181-186.	1.2	180

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37	Strain engineering of selective chemical adsorption on monolayer MoS₂. Nanoscale, 2014, 6, 5156-5161.	2.8	177
38	Auxetic and Ferroelastic Borophane: A Novel 2D Material with Negative Possionâ€™s Ratio and Switchable Dirac Transport Channels. Nano Letters, 2016, 16, 7910-7914.	4.5	176
39	Dots versus Antidots: Computational Exploration of Structure, Magnetism, and Half-Metallicity in Boronâ^'Nitride Nanostructures. Journal of the American Chemical Society, 2009, 131, 17354-17359.	6.6	174
40	Hydrogenated borophene as a stable two-dimensional Dirac material with an ultrahigh Fermi velocity. Physical Chemistry Chemical Physics, 2016, 18, 27284-27289.	1.3	167
41	Tuning oxygen vacancies in two-dimensional iron-cobalt oxide nanosheets through hydrogenation for enhanced oxygen evolution activity. Nano Research, 2018, 11, 3509-3518.	5.8	167
42	Lithiumâ€Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage. Advanced Functional Materials, 2009, 19, 265-271.	7.8	156
43	Manipulating the Solvation Structure of Nonflammable Electrolyte and Interface to Enable Unprecedented Stability of Graphite Anodes beyond 2 Years for Safe Potassiumâ€Ion Batteries. Advanced Materials, 2021, 33, e2006313.	11.1	155
44	Tuning the Intermolecular Electron Transfer of Low-Dimensional and Metal-Free BCN/C₆₀ Electrocatalysts via Interfacial Defects for Efficient Hydrogen and Oxygen Electrochemistry. Journal of the American Chemical Society, 2021, 143, 1203-1215.	6.6	140
45	Mo-based 2D MOF as a highly efficient electrocatalyst for reduction of N₂ to NH₃: a density functional theory study. Journal of Materials Chemistry A, 2019, 7, 14510-14518.	5.2	139
46	Activating Catalytic Inert Basal Plane of Molybdenum Disulfide to Optimize Hydrogen Evolution Activity via Defect Doping and Strain Engineering. Journal of Physical Chemistry C, 2016, 120, 16761-16766.	1.5	138
47	Metallic and Carbon Nanotube-Catalyzed Coupling of Hydrogenation in Magnesium. Journal of the American Chemical Society, 2007, 129, 15650-15654.	6.6	131
48	Computational screening of two-dimensional coordination polymers as efficient catalysts for oxygen evolution and reduction reaction. Journal of Catalysis, 2017, 352, 579-585.	3.1	130
49	Electronic and optical properties of lead-free hybrid double perovskites for photovoltaic and optoelectronic applications. Scientific Reports, 2019, 9, 718.	1.6	130
50	Highâ€Performance Perovskite Composite Electrocatalysts Enabled by Controllable Interface Engineering. Small, 2021, 17, e2101573.	5.2	128
51	Metal-free graphitic carbon nitride as mechano-catalyst for hydrogen evolution reaction. Journal of Catalysis, 2015, 332, 149-155.	3.1	127
52	Single tungsten atom supported on N-doped graphyne as a high-performance electrocatalyst for nitrogen fixation under ambient conditions. Physical Chemistry Chemical Physics, 2019, 21, 1546-1551.	1.3	126
53	Transition metal dichalcogenides bilayer single crystals by reverse-flow chemical vapor epitaxy. Nature Communications, 2019, 10, 598.	5.8	124
54	Atomically embedded asymmetrical dual-metal dimers on N-doped graphene for ultra-efficient nitrogen reduction reaction. Journal of Catalysis, 2020, 388, 77-83.	3.1	123

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55	A Directional Synthesis for Topological Defect in Carbon. CheM, 2020, 6, 2009-2023.	5.8	120
56	The Role of Ti as a Catalyst for the Dissociation of Hydrogen on a Mg(0001) Surface. Journal of Physical Chemistry B, 2005, 109, 18037-18041.	1.2	113
57	Tailoring the Interfacial Interactions of van der Waals 1T-MoS₂/C₆₀ Heterostructures for High-Performance Hydrogen Evolution Reaction Electrocatalysis. Journal of the American Chemical Society, 2020, 142, 17923-17927.	6.6	112
58	Controllable CO2 electrocatalytic reduction via ferroelectric switching on single atom anchored In2Se3 monolayer. Nature Communications, 2021, 12, 5128.	5.8	110
59	A single boron atom doped boron nitride edge as a metal-free catalyst for N₂ fixation. Physical Chemistry Chemical Physics, 2019, 21, 1110-1116.	1.3	107
60	C-BN Single-Walled Nanotubes from Hybrid Connection of BN/C Nanoribbons: Prediction by ab initio Density Functional Calculations. Journal of the American Chemical Society, 2009, 131, 1682-1683.	6.6	106
61	Hydrogen Spillover Mechanism on a Pd-Doped Mg Surface as Revealed by ab initio Density Functional Calculation. Journal of the American Chemical Society, 2007, 129, 10201-10204.	6.6	105
62	Carbon nanodot decorated graphitic carbon nitride: new insights into the enhanced photocatalytic water splitting from ab initio studies. Physical Chemistry Chemical Physics, 2015, 17, 31140-31144.	1.3	105
63	Widely tunable and anisotropic charge carrier mobility in monolayer tin(<scp>ii</scp>) selenide using biaxial strain: a first-principles study. Journal of Materials Chemistry C, 2017, 5, 1247-1254.	2.7	104
64	Computational Dissection of Two-Dimensional Rectangular Titanium Mononitride TiN: Auxetics and Promises for Photocatalysis. Nano Letters, 2017, 17, 4466-4472.	4.5	104
65	Gas sensing and capturing based on twoâ€dimensional layered materials: Overview from theoretical perspective. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1361.	6.2	101
66	Twoâ€Dimensional Boron Hydride Sheets: High Stability, Massless Dirac Fermions, and Excellent Mechanical Properties. Angewandte Chemie - International Edition, 2016, 55, 10292-10295.	7.2	100
67	Predicting Single-Layer Technetium Dichalcogenides (TcX₂, X = S, Se) with Promising Applications in Photovoltaics and Photocatalysis. ACS Applied Materials & Interfaces, 2016, 8, 5385-5392.	4.0	100
68	Single Pt atom decorated graphitic carbon nitride as an efficient photocatalyst for the hydrogenation of nitrobenzene into aniline. Nano Research, 2019, 12, 1817-1823.	5.8	100
69	Porous Polyethersulfone-Supported Zeolitic Imidazolate Framework Membranes for Hydrogen Separation. Journal of Physical Chemistry C, 2012, 116, 13264-13270.	1.5	96
70	Nanosheets Co₃O₄ Interleaved with Graphene for Highly Efficient Oxygen Reduction. ACS Applied Materials & Interfaces, 2015, 7, 21373-21380.	4.0	96
71	Stable Copper Nanoparticle Photocatalysts for Selective Epoxidation of Alkenes with Visible Light. ACS Catalysis, 2017, 7, 4975-4985.	5.5	96
72	Mg-Based Nanocomposites with High Capacity and Fast Kinetics for Hydrogen Storage. Journal of Physical Chemistry B, 2006, 110, 11697-11703.	1.2	95

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73	Modelling carbon membranes for gas and isotope separation. Physical Chemistry Chemical Physics, 2013, 15, 4832.	1.3	95
74	Twoâ€Dimensional Boron Hydride Sheets: High Stability, Massless Dirac Fermions, and Excellent Mechanical Properties. Angewandte Chemie, 2016, 128, 10448-10451.	1.6	94
75	Understanding the activity and selectivity of single atom catalysts for hydrogen and oxygen evolution via ab initial study. Catalysis Science and Technology, 2018, 8, 996-1001.	2.1	94
76	An Unusual Red Carbon Nitride to Boost the Photoelectrochemical Performance of Wide Bandgap Photoanodes. Advanced Functional Materials, 2018, 28, 1805698.	7.8	94
77	Strong Coupling of MoS₂ Nanosheets and Nitrogenâ€Doped Graphene for Highâ€Performance Pseudocapacitance Lithium Storage. Small, 2018, 14, e1704410.	5.2	89
78	Understanding the Roles of Oxygen Vacancies in Hematiteâ€Based Photoelectrochemical Processes. Angewandte Chemie, 2019, 131, 1042-1046.	1.6	89
79	Tailoring Crystal Structure of FA_{0.83}Cs_{0.17}PbI₃ Perovskite Through Guanidinium Doping for Enhanced Performance and Tunable Hysteresis of Planar Perovskite Solar Cells. Advanced Functional Materials, 2019, 29, 1806479.	7.8	87
80	First principle studies of zigzag AlN nanoribbon. Chemical Physics Letters, 2009, 469, 183-185.	1.2	86
81	Dualâ€Ionâ€Diffusion Induced Degradation in Leadâ€Free Cs₂AgBiBr₆ Double Perovskite Solar Cells. Advanced Functional Materials, 2020, 30, 2002342.	7.8	86
82	Endohedral metallofullerenes (M@C60) as efficient catalysts for highly active hydrogen evolution reaction. Journal of Catalysis, 2017, 354, 231-235.	3.1	84
83	First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. Physical Review Letters, 2017, 119, 016403.	2.9	84
84	2Dâ€“3D Mixed Organicâ€“Inorganic Perovskite Layers for Solar Cells with Enhanced Efficiency and Stability Induced by n-Propylammonium Iodide Additives. ACS Applied Materials & Interfaces, 2019, 11, 29753-29764.	4.0	83
85	Spin-polarization and ferromagnetism of graphitic carbon nitride materials. Journal of Materials Chemistry C, 2013, 1, 6265.	2.7	82
86	Identifying Copper Vacancies and Their Role in the CuO Based Photocathode for Water Splitting. Angewandte Chemie - International Edition, 2019, 58, 17604-17609.	7.2	82
87	Asymmetrically Decorated, Doped Porous Graphene As an Effective Membrane for Hydrogen Isotope Separation. Journal of Physical Chemistry C, 2012, 116, 6672-6676.	1.5	81
88	Two-dimensional GeP₃ as a high capacity electrode material for Li-ion batteries. Physical Chemistry Chemical Physics, 2017, 19, 25886-25890.	1.3	81
89	A density functional theory study on CO2 capture and activation by graphene-like boron nitride with boron vacancy. Catalysis Today, 2011, 175, 271-275.	2.2	80
90	Single layer lead iodide: computational exploration of structural, electronic and optical properties, strain induced band modulation and the role of spinâ€“orbital-coupling. Nanoscale, 2015, 7, 15168-15174.	2.8	80

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91	Gradientâ€Concentration Design of Stable Coreâ€“Shell Nanostructure for Acidic Oxygen Reduction Electrocatalysis. Advanced Materials, 2020, 32, e2003493.	11.1	79
92	Electric field controlled CO₂capture and CO₂/N₂separation on MoS₂monolayers. Nanoscale, 2017, 9, 19-24.	2.8	78
93	Atomically Dispersed Heteronuclear Dualâ€Atom Catalysts: A New Rising Star in Atomic Catalysis. Small, 2022, 18, e2106091.	5.2	78
94	Carbon Dioxide Capture and Gas Separation on B₈₀ Fullerene. Journal of Physical Chemistry C, 2014, 118, 2170-2177.	1.5	77
95	Electrochemical reduction of carbon dioxide on precise number of Fe atoms anchored graphdiyne. Journal of CO2 Utilization, 2020, 37, 272-277.	3.3	76
96	Predicting Two-Dimensional C₃B/C₃N van der Waals pâ€“n Heterojunction with Strong Interlayer Electron Coupling and Enhanced Photocurrent. Journal of Physical Chemistry Letters, 2018, 9, 858-862.	2.1	74
97	Novel two-dimensional MOF as a promising single-atom electrocatalyst for CO2 reduction: A theoretical study. Applied Surface Science, 2020, 500, 143993.	3.1	74
98	Plasma-induced on-surface sulfur vacancies in NiCo₂S₄ enhance the energy storage performance of supercapatteries. Journal of Materials Chemistry A, 2020, 8, 9278-9291.	5.2	73
99	Strong affinity of polysulfide intermediates to multi-functional binder for practical application in lithiumâ€“sulfur batteries. Nano Energy, 2016, 26, 722-728.	8.2	72
100	Hindered Formation of Photoinactive Î´-FAPbI₃ Phase and Hysteresis-Free Mixed-Cation Planar Heterojunction Perovskite Solar Cells with Enhanced Efficiency via Potassium Incorporation. Journal of Physical Chemistry Letters, 2018, 9, 2113-2120.	2.1	72
101	Two-Dimensional Titanium Carbonitride Mxene for High-Performance Sodium Ion Batteries. ACS Applied Nano Materials, 2018, 1, 6854-6863.	2.4	71
102	Metal-doped graphitic carbon nitride (g-C3N4) as selective NO2 sensors: A first-principles study. Applied Surface Science, 2018, 455, 1116-1122.	3.1	71
103	Single-atom supported on graphene grain boundary as an efficient electrocatalyst for hydrogen evolution reaction. Chemical Engineering Science, 2019, 194, 58-63.	1.9	71
104	Computation-Aided Design of Single-Atom Catalysts for One-Pot CO₂ Capture, Activation, and Conversion. ACS Applied Materials & Interfaces, 2018, 10, 36866-36872.	4.0	70
105	A water-dielectric capacitor using hydrated graphene oxide film. Journal of Materials Chemistry, 2012, 22, 21085.	6.7	68
106	Ab initio studies of hydrogen desorption from low index magnesium hydride surface. Surface Science, 2006, 600, 1854-1859.	0.8	67
107	Single Layer Bismuth Iodide: Computational Exploration of Structural, Electrical, Mechanical and Optical Properties. Scientific Reports, 2015, 5, 17558.	1.6	67
108	H₂ purification by functionalized graphdiyne â€“ role of nitrogen doping. Journal of Materials Chemistry A, 2015, 3, 6767-6771.	5.2	67

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109	Ultra-dense carbon defects as highly active sites for oxygen reduction catalysis. CheM, 2022, 8, 2715-2733.	5.8	66
110	Predicting Novel 2D MB₂ (M = Ti, Hf, V, Nb, Ta) Monolayers with Ultrafast Dirac Transport Channel and Electron-Orbital Controlled Negative Poissonâ€™s Ratio. Journal of Physical Chemistry Letters, 2019, 10, 2567-2573.	2.1	65
111	Surfaceâ€Dependent Intermediate Adsorption Modulation on Iridiumâ€Modified Black Phosphorus Electrocatalysts for Efficient pHâ€Universal Water Splitting. Advanced Materials, 2021, 33, e2104638.	11.1	65
112	High capacity and reversible hydrogen storage on two dimensional C 2 N monolayer membrane. International Journal of Hydrogen Energy, 2018, 43, 9895-9901.	3.8	64
113	Controlling the Interfacial Charge Polarization of MOF-Derived 0Dâ€“2D vdW Architectures as a Unique Strategy for Bifunctional Oxygen Electrocatalysis. ACS Applied Materials & Interfaces, 2022, 14, 3919-3929.	4.0	63
114	A density functional theory study of CO2 and N2 adsorption on aluminium nitride single walled nanotubes. Journal of Materials Chemistry, 2010, 20, 10426.	6.7	62
115	Electrocatalytically Switchable CO₂ Capture: First Principle Computational Exploration of Carbon Nanotubes with Pyridinic Nitrogen. ChemSusChem, 2014, 7, 435-441.	3.6	62
116	First-Principle Studies of the Formation and Diffusion of Hydrogen Vacancies in Magnesium Hydride. Journal of Physical Chemistry C, 2007, 111, 8360-8365.	1.5	61
117	Predicting a new class of metal-organic frameworks as efficient catalyst for bi-functional oxygen evolution/reduction reactions. Journal of Catalysis, 2018, 367, 206-211.	3.1	61
118	Versatile Single-Layer Sodium Phosphidostannate(II): Strain-Tunable Electronic Structure, Excellent Mechanical Flexibility, and an Ideal Gap for Photovoltaics. Journal of Physical Chemistry Letters, 2015, 6, 2682-2687.	2.1	60
119	Ultrathin Cobaltosic Oxide Nanosheets as an Effective Sulfur Encapsulation Matrix with Strong Affinity Toward Polysulfides. ACS Applied Materials & Interfaces, 2017, 9, 4320-4325.	4.0	59
120	Simplest MOF Units for Effective Photodriven Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 9159-9166.	6.6	59
121	Reversible gas capture using a ferroelectric switch and 2D molecule multiferroics on the In₂Se₃ monolayer. Journal of Materials Chemistry A, 2020, 8, 7331-7338.	5.2	59
122	Sodium and Lithium Storage Properties of Spray-Dried Molybdenum Disulfide-Graphene Hierarchical Microspheres. Scientific Reports, 2015, 5, 11989.	1.6	58
123	Atomically dispersed asymmetric Cuâ€“B pair on 2D carbon nitride synergistically boosts the conversion of CO into C₂ products. Journal of Materials Chemistry A, 2020, 8, 599-606.	5.2	58
124	Fabricating highly efficient heterostructured CuBi₂O₄ photocathodes for unbiased water splitting. Journal of Materials Chemistry A, 2020, 8, 2498-2504.	5.2	57
125	Electronic Functionality in Graphene-Based Nanoarchitectures: Discovery and Design via First-Principles Modeling. Journal of Physical Chemistry Letters, 2011, 2, 73-80.	2.1	56
126	Van der Waals-corrected density functional theory: benchmarking for hydrogenâ€“nanotube and nanotubeâ€“nanotube interactions. Nanotechnology, 2005, 16, 2118-2123.	1.3	55

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127	Catalytic Effects of Subsurface Carbon in the Chemisorption of Hydrogen on a Mg(0001) Surface:Â an Ab-initio Study. Journal of Physical Chemistry B, 2006, 110, 1814-1819.	1.2	55
128	Combined electrophoretic depositionâ€“anodization method to fabricate reduced graphene oxideâ€“TiO2 nanotube films. RSC Advances, 2012, 2, 8164.	1.7	55
129	Distorted Janus Transition Metal Dichalcogenides: Stable Two-Dimensional Materials with Sizable Band Gap and Ultrahigh Carrier Mobility. Journal of Physical Chemistry C, 2018, 122, 19153-19160.	1.5	55
130	Moltenâ€Saltâ€Mediated Synthesis of an Atomic Nickel Coâ€catalyst on TiO₂ for Improved Photocatalytic H₂ Evolution. Angewandte Chemie, 2020, 132, 7297-7301.	1.6	55
131	A zinc bromine â€œsupercapatteryâ€•system combining triple functions of capacitive, pseudocapacitive and battery-type charge storage. Materials Horizons, 2020, 7, 495-503.	6.4	54
132	Adsorption of Carbon Dioxide and Nitrogen on Single-Layer Aluminum Nitride Nanostructures Studied by Density Functional Theory. Journal of Physical Chemistry C, 2010, 114, 7846-7849.	1.5	53
133	First-Principle Study of Adsorption of Hydrogen on Ti-Doped Mg(0001) Surface. Journal of Physical Chemistry B, 2006, 110, 21747-21750.	1.2	52
134	Gas Protection of Two-Dimensional Nanomaterials from High-Energy Impacts. Scientific Reports, 2016, 6, 35532.	1.6	52
135	Computational screening of MN₄ (M = Tiâ€“Cu) based metal organic frameworks for CO₂ reduction using the d-band centre as a descriptor. Nanoscale, 2020, 12, 6188-6194.	2.8	52
136	Novel Excitonic Solar Cells in Phosphoreneâ€“TiO₂ Heterostructures with Extraordinary Charge Separation Efficiency. Journal of Physical Chemistry Letters, 2016, 7, 1880-1887.	2.1	51
137	In-plane graphene/boron-nitride heterostructures as an efficient metal-free electrocatalyst for the oxygen reduction reaction. Nanoscale, 2016, 8, 14084-14091.	2.8	51
138	Versatile two-dimensional silicon diphosphide (SiP₂) for photocatalytic water splitting. Nanoscale, 2018, 10, 6369-6374.	2.8	51
139	Firstâ€Principles Study of Electrocatalytically Reversible CO₂ Capture on Grapheneâ€like C₃N. ChemPhysChem, 2018, 19, 2788-2795.	1.0	51
140	Silicon-doped graphene edges: an efficient metal-free catalyst for the reduction of CO₂ into methanol and ethanol. Catalysis Science and Technology, 2019, 9, 6800-6807.	2.1	51
141	Predicting a new phase (Tâ€²â€²) of two-dimensional transition metal di-chalcogenides and strain-controlled topological phase transition. Nanoscale, 2016, 8, 4969-4975.	2.8	50
142	Ab initio atomistic insights into lead-free formamidinium based hybrid perovskites for photovoltaics and optoelectronics. Computational Materials Science, 2019, 169, 109118.	1.4	50
143	Reversible Intercalation of Multivalent Al³⁺ Ions into Potassiumâ€Rich Cryptomelane Nanowires for Aqueous Rechargeable Alâ€Ion Batteries. ChemSusChem, 2019, 12, 3753-3760.	3.6	50
144	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB₃monolayer. Nanoscale Horizons, 2021, 6, 43-48.	4.1	50

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145	Leaf-inspired design of mesoporous Sb2S3/N-doped Ti3C2Tx composite towards fast sodium storage. Science China Chemistry, 2021, 64, 964-973.	4.2	50
146	Doped phosphorene for hydrogen capture: A DFT study. Applied Surface Science, 2018, 433, 249-255.	3.1	48
147	First-principles screening of novel ferroelectric MXene phases with a large piezoelectric response and unusual auxeticity. Nanoscale, 2020, 12, 21291-21298.	2.8	48
148	Computational Design and Experimental Validation of the Optimal Bimetal-Doped SrCoO_{3â^'Î´} Perovskite as Solid Oxide Fuel Cell Cathode. Journal of the American Chemical Society, 2021, 143, 9507-9514.	6.6	48
149	Insights into the nature of the coupling interactions between uracil corrosion inhibitors and copper: A DFT and molecular dynamics study. Corrosion Science, 2012, 61, 101-110.	3.0	47
150	Moleculeâ€Induced Conformational Change in Boron Nitride Nanosheets with Enhanced Surface Adsorption. Advanced Functional Materials, 2016, 26, 8202-8210.	7.8	47
151	WO₃ nanolayer coated 3D-graphene/sulfur composites for high performance lithium/sulfur batteries. Journal of Materials Chemistry A, 2019, 7, 4596-4603.	5.2	47
152	Development of cross-linked dextrin as aqueous binders for silicon based anodes. Journal of Power Sources, 2020, 450, 227671.	4.0	47
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