Aijun Du

List of Publications by Year
in descending order

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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	Vacancy engineering of oxidized Nb2CTx MXenes for a biased nitrogen fixation. Green Energy and Environment, 2023, 8, 1185-1194.	4.7	11
2	B-incorporated, N-doped hierarchically porous carbon nanosheets as anodes for boosted potassium storage capability. Chinese Chemical Letters, 2022, 33, 480-485.	4.8	15
3	Coupling Fe3O4/Fe1-xS@Carbon with carbon-coated MoS2 nanosheets as a superior anode for sodium-ion batteries. Chemical Engineering Journal, 2022, 427, 131652.	6.6	10
4	In-situ conversion growth of carbon-coated MoS2/N-doped carbon nanotubes as anodes with superior capacity retention for sodium-ion batteries. Journal of Materials Science and Technology, 2022, 102, 8-15.	5.6	16
5	Carbon-coated MoS2 nanosheets@CNTs-Ti3C2 MXene quaternary composite with the superior rate performance for sodium-ion batteries. Journal of Materials Science and Technology, 2022, 100, 101-109.	5.6	29
6	Nanostructure Shape-Effects in ZnO heterogeneous photocatalysis. Journal of Colloid and Interface Science, 2022, 606, 588-599.	5.0	32
7	Co Nanoparticles Encapsulated in Nâ€Doped Carbon Nanotubes Grafted CNTs as Electrocatalysts for Enhanced Oxygen Reduction Reaction. Advanced Materials Interfaces, 2022, 9, .	1.9	8
8	hcp-phased Ni nanoparticles with generic catalytic hydrogenation activities toward different functional groups. Science China Materials, 2022, 65, 1252-1261.	3.5	5
9	Computational screening of single-atom alloys TM@Ru(0001) for enhanced electrochemical nitrogen reduction reaction. Journal of Materials Chemistry A, 2022, 10, 6204-6215.	5.2	33
10	Wavelength-Specific Product Desorption as a Key to Raising Nitrile Yield of Primary Alcohol Ammoxidation over Illuminated Pd Nanoparticles. ACS Catalysis, 2022, 12, 2280-2289.	5.5	17
11	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
12	Adina Rubellaâ€Like Microsized SiO@Nâ€Doped Carbon Grafted with Nâ€Doped Carbon Nanotubes as Anodes for Highâ€Performance Lithium Storage. Small Science, 2022, 2, .	5.8	33
13	Green ammonia synthesis using CeO₂/RuO₂ nanolayers on vertical graphene catalyst via electrochemical route in alkaline electrolyte. Nanoscale, 2022, 14, 1395-1408.	2.8	11
14	Atomically Dispersed Heteronuclear Dualâ€Atom Catalysts: A New Rising Star in Atomic Catalysis. Small, 2022, 18, e2106091.	5.2	78
15	Revealing the Potential of Ternary Medium-Entropy Alloys as Exceptional Electrocatalysts toward Nitrogen Reduction: An Example of Heusler Alloys. ACS Applied Materials & Interfaces, 2022, 14, 15235-15242.	4.0	15
16	Kâ€Functionalized Carbon Quantum Dotsâ€Induced Interface Assembly of Carbon Nanocages for Ultrastable Potassium Storage Performance. Small Methods, 2022, 6, e2101627.	4.6	12
17	Nitrateâ€toâ€Ammonia Conversion at an InSnâ€Enriched Liquidâ€Metal Electrode. Angewandte Chemie - International Edition, 2022, 61, .	7.2	34
18	Hydrogen-Intercalated 2D Magnetic Bilayer: Controlled Magnetic Phase Transition and Half-Metallicity via Ferroelectric Switching. ACS Applied Materials & Interfaces, 2022, 14, 1800-1806.	4.0	20

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19	N/P-Doped MoS₂ Monolayers as Promising Materials for Controllable CO₂ Capture and Separation under Reduced Electric Fields: A Theoretical Modeling. Journal of Physical Chemistry C, 2022, 126, 203-211.	1.5	6
20	Controllable Acceleration and Deceleration of Charge Carrier Transport in Metalâ€Halide Perovskite Singleâ€Crystal by Csâ€Cation Induced Bandgap Engineering. Small, 2022, 18, e2107680.	5.2	3
21	2D/2D Black Phosphorus/Nickel Hydroxide Heterostructures for Promoting Oxygen Evolution via Electronic Structure Modulation and Surface Reconstruction. Advanced Energy Materials, 2022, 12, .	10.2	37
22	Versatile Gold Telluride Iodide Monolayer as a Potential Photocatalyst for Water Splitting. Nanomaterials, 2022, 12, 1915.	1.9	4
23	First-Principles Study of the Enhanced Magnetic Anisotropy and Transition Temperature in a CrSe₂ Monolayer via Hydrogenation. ACS Applied Electronic Materials, 2022, 4, 3240-3245.	2.0	18
24	Pumpkin-like MoP-MoS2@Aspergillus niger spore-derived N-doped carbon heterostructure for enhanced potassium storage. Journal of Energy Chemistry, 2022, 72, 479-486.	7.1	14
25	Switchable topological phase transition and nonlinear optical properties in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>ReC</mml:mi><mml:mn>2</mml:mn></m mathvariant="normal">H</mml:mi></mml:mrow></mml:math> monolayer. Physical Review B, 2022, 105, .	3.2	6
26	Theoretical Study of a Novel WSi₂N₄/MoSi₂N₄ Heterostructure with Ultrafast Carrier Transport. Journal of Physical Chemistry C, 2022, 126, 11380-11388.	1.5	20
27	Superb storage and energy saving separation of hydrocarbon gases in boron nitride nanosheets via a mechanochemical process. Materials Today, 2022, 57, 26-34.	8.3	6
28	Ultra-dense carbon defects as highly active sites for oxygen reduction catalysis. CheM, 2022, 8, 2715-2733.	5.8	66
29	High capacity and mobility in germanium sulfide/graphene (GeS/Gr) van der Waals heterostructure as anode materials for sodiumâ€"ion batteries: A first-principles investigation. Applied Surface Science, 2021, 536, 147779.	3.1	15
30	Theoretical insights into the performance of single and double transition metal atoms doped on N-graphenes for N2 electroreduction. Applied Surface Science, 2021, 537, 148012.	3.1	27
31	First principles studies of mononuclear and dinuclear Pacman complexes for electrocatalytic reduction of CO2. Catalysis Science and Technology, 2021, 11, 637-645.	2.1	3
32	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB₃monolayer. Nanoscale Horizons, 2021, 6, 43-48.	4.1	50
33	Two-dimensional vanadium tetrafluoride with antiferromagnetic ferroelasticity and bidirectional negative Poisson's ratio. Journal of Materials Chemistry C, 2021, 9, 95-100.	2.7	18
34	<scp>N₂</scp> electrochemical reduction on two dimensional transition metal monoborides: A density functional theory study. International Journal of Quantum Chemistry, 2021, 121, e26548.	1.0	4
35	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
36	Ultrasmall SnO₂ nanocrystals sandwiched into polypyrrole and Ti₃C₂T_x MXene for highly effective sodium storage. Materials Chemistry Frontiers, 2021, 5, 825-833.	3.2	25

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37	Exploring Aluminumâ€Ion Insertion into Magnesiumâ€Doped Manjiroite (MnO₂) Nanorods in Aqueous Solution. ChemElectroChem, 2021, 8, 1048-1054.	1.7	9
38	Integrating SnS₂ Quantum Dots with Nitrogen-Doped Ti₃C₂T_x MXene Nanosheets for Robust Sodium Storage Performance. ACS Applied Energy Materials, 2021, 4, 846-854.	2.5	40
39	First-principles prediction of polar half-metallicity and out-of-plane piezoelectricity in two-dimensional quintuple layered cobalt selenide. Journal of Materials Chemistry C, 2021, 9, 12046-12050.	2.7	11
40	Unlocking the potential of ruthenium catalysts for nitrogen fixation with subsurface oxygen. Journal of Materials Chemistry A, 2021, 9, 6575-6582.	5.2	14
41	Tuning CO binding strengthviaengineering the copper/borophene interface for highly efficient conversion of CO into ethanol. Journal of Materials Chemistry A, 2021, 9, 13192-13199.	5.2	23
42	Prediction of two-dimensional ferroelectric metal Mxenes. Journal of Materials Chemistry C, 2021, 9, 11343-11348.	2.7	15
43	First-principles prediction of ferroelasticity tuned anisotropic auxeticity and carrier mobility in two-dimensional AgO. Journal of Materials Chemistry C, 2021, 9, 3155-3160.	2.7	11
44	Exploring Aluminumâ€Ion Insertion into Magnesiumâ€Doped Manjiroite (MnO 2) Nanorods in Aqueous Solution. ChemElectroChem, 2021, 8, 995-995.	1.7	0
45	Thermal Reductive Perforation of Graphene Cathode for Highâ€Performance Aluminumâ€Ion Batteries. Advanced Functional Materials, 2021, 31, 2010569.	7.8	41
46	Leaf-inspired design of mesoporous Sb2S3/N-doped Ti3C2Tx composite towards fast sodium storage. Science China Chemistry, 2021, 64, 964-973.	4.2	50
47	Sn²⁺-Regulated Synthesis of a Bone-like Fe₃O₄@N-Doped Carbon Composite as the Anode for High-Performance Lithium Storage. ACS Applied Energy Materials, 2021, 4, 3785-3793.	2.5	8
48	Regulating the interfacial behavior of carbon nanotubes for fast lithium storage. Electrochimica Acta, 2021, 388, 138591.	2.6	7
49	A Highly Efficient Conjoinedâ€twin Porphyrinâ€based Complex for the Electrochemical Reduction of CO to Ethanol. ChemNanoMat, 2021, 7, 935-941.	1.5	2
50	Highâ€Performance Perovskite Composite Electrocatalysts Enabled by Controllable Interface Engineering. Small, 2021, 17, e2101573.	5.2	128
51	Unravelling the Reaction Mechanisms of N₂ Fixation on Molybdenum Nitride: A Full DFT Study from the Pristine Surface to Heteroatom Anchoring. ChemSusChem, 2021, 14, 3257-3266.	3.6	22
52	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
53	Boron-rich boron nitride nanomaterials as efficient metal-free catalysts for converting CO2 into valuable fuel. Applied Surface Science, 2021, 555, 149652.	3.1	20
54	Controllable CO2 electrocatalytic reduction via ferroelectric switching on single atom anchored In2Se3 monolayer. Nature Communications, 2021, 12, 5128.	5.8	110

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55	Purely one-dimensional ferroelectricity and antiferroelectricity from van der Waals niobium oxide trihalides. Npj Computational Materials, 2021, 7, .	3.5	14
56	Rhodium-molybdenum oxide electrocatalyst with dual active sites for electrochemical ammonia synthesis under neutral pH condition. Journal of Electroanalytical Chemistry, 2021, 896, 115157.	1.9	10
57	CO₂ Capture, Separation and Reduction on Boronâ€Doped MoS₂, MoSe₂ and Heterostructures with Different Doping Densities: A Theoretical Study. ChemPhysChem, 2021, 22, 2392-2400.	1.0	4
58	Predicting MnB6 monolayer with room temperature ferromagnetism and high magnetic anisotropy. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 134, 114930.	1.3	6
59	Interfacing 2D VS2 with Janus MoSSe: Antiferromagnetic electric polarization and charge transfer driven Half-metallicity. Applied Surface Science, 2021, 570, 151129.	3.1	4
60	Techniques enabling inorganic materials into wearable fiber/yarn and flexible lithium-ion batteries. Energy Storage Materials, 2021, 43, 62-84.	9.5	25
61	Numerical investigation of microstructure and failure of lithiated silicon under biaxial tension. Computational Materials Science, 2021, 200, 110764.	1.4	0
62	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
63	Graphynes as emerging 2D-platforms for electronic and energy applications: a computational perspective. Materials Chemistry Frontiers, 2021, 5, 6392-6412.	3.2	17
64	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
65	Controllable Polarization and Doping in Ferroelectric In₂Se₃ Monolayers and Heterobilayers via Intrinsic Defect Engineering. Journal of Physical Chemistry C, 2021, 125, 24648-24654.	1.5	12
66	Two-Dimensional Janus Antimony Selenium Telluride with Large Rashba Spin Splitting and High Electron Mobility. ACS Omega, 2021, 6, 31919-31925.	1.6	5
67	Cobalt porphyrin supported on graphene/Ni (111) surface: Enhanced oxygen evolution/reduction reaction and the role of electron coupling. Catalysis Today, 2020, 351, 113-118.	2.2	28
68	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
69	Strain engineering of selective chemical adsorption on monolayer black phosphorous. Applied Surface Science, 2020, 503, 144033.	3.1	25
70	Functionalized boron nitride monolayers as promising materials for uranyl ion capture: A first-principles study. Journal of Molecular Structure, 2020, 1200, 127080.	1.8	4
71	Highly stable two-dimensional gold selenide with large in-plane anisotropy and ultrahigh carrier mobility. Nanoscale Horizons, 2020, 5, 366-371.	4.1	28
72	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

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73	Fabricating highly efficient heterostructured CuBi₂O₄ photocathodes for unbiased water splitting. Journal of Materials Chemistry A, 2020, 8, 2498-2504.	5.2	57
74	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msup><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:mi mathvariant="normal">u</mml:mi></mml:mrow><mml:mrow><mml:mi>Î´</mml:mi><mml:mo>+</mml:mo></mml:mrow></mml:msup> active sites stabilization through Mott-Schottky effect for promoting highly efficient conversion of carbon monoxide into n-propanol. Journal of Catalysis, 2020, 382, 49-56.	3.1	27
75	Two-dimensional heterojunction SnS2/SnO2 photoanode with excellent photoresponse up to near infrared region. Solar Energy Materials and Solar Cells, 2020, 207, 110342.	3.0	13
76	Electrochemical reduction of carbon dioxide on precise number of Fe atoms anchored graphdiyne. Journal of CO2 Utilization, 2020, 37, 272-277.	3.3	76
77	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
78	Development of cross-linked dextrin as aqueous binders for silicon based anodes. Journal of Power Sources, 2020, 450, 227671.	4.0	47
79	Borophene: A Metalâ€free and Metallic Electrocatalyst for Efficient Converting CO₂ into CH₄. ChemCatChem, 2020, 12, 1483-1490.	1.8	29
80	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI₃/CrGeTe₃ Nanostructures for Spintronics. ACS Applied Nano Materials, 2020, 3, 1282-1288.	2.4	47
81	An Intrinsically Nonâ€flammable Electrolyte for Highâ€Performance Potassium Batteries. Angewandte Chemie - International Edition, 2020, 59, 3638-3644.	7.2	211
82	First-principles study of a Mn-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:n monolayer: Coexistence of ferromagnetism and ferroelectricity with robust half-metallicity and enhanced polarization. Physical Review B, 2020, 102, .	1.1	18
83	Solvent Effect on Supramolecular Self-Assembly of Chlorophylls a on Chemically Reduced Graphene Oxide. Langmuir, 2020, 36, 13575-13582.	1.6	9
84	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
85	2D atomic crystal molecular superlattices by soft plasma intercalation. Nature Communications, 2020, 11, 5960.	5.8	36
86	Strain induced variation of PFOS adsorption on pristine and defected phosphorene: A DFT study. Applied Surface Science, 2020, 532, 147452.	3.1	7
87	Single Copper Atoms Supported on ZnS as an Efficient Catalyst for Electrochemical Reduction of CO to CH₃OH. ChemNanoMat, 2020, 6, 1806-1811.	1.5	9
88	First-principles screening of novel ferroelectric MXene phases with a large piezoelectric response and unusual auxeticity. Nanoscale, 2020, 12, 21291-21298.	2.8	48
89	Tuning band alignment and optical properties of 2D van der Waals heterostructure via ferroelectric polarization switching. Frontiers of Physics, 2020, 15, 1.	2.4	20
90	Dualâ€Ionâ€Diffusion Induced Degradation in Leadâ€Free Cs₂AgBiBr₆ Double Perovskite Solar Cells. Advanced Functional Materials, 2020, 30, 2002342.	7.8	86

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91	Tunable magnetic anisotropy in 2D magnets via molecular adsorption. Journal of Materials Chemistry C, 2020, 8, 14948-14953.	2.7	26
92	Direct conversion of metal organic frameworks into ultrafine phosphide nanocomposites in multicomponent plasma for wide pH hydrogen evolution. Journal of Materials Chemistry A, 2020, 8, 10402-10408.	5.2	15
93	In Situ Formation of Oxygen Vacancies Achieving Nearâ€Complete Charge Separation in Planar BiVO₄ Photoanodes. Advanced Materials, 2020, 32, e2001385.	11.1	236
94	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
95	The importance of atomic charge distributions of solid boron material in N2 electrochemical reduction. Applied Surface Science, 2020, 526, 146606.	3.1	13
96	Potassium Doping to Enhance Green Photoemission of Lightâ€Emitting Diodes Based on CsPbBr₃ Perovskite Nanocrystals. Advanced Optical Materials, 2020, 8, 2000742.	3.6	32
97	Remarkably improved oxygen evolution reaction activity of cobalt oxides by an Fe ion solution immersion process. Inorganic Chemistry Frontiers, 2020, 7, 3327-3339.	3.0	29
98	A Directional Synthesis for Topological Defect in Carbon. CheM, 2020, 6, 2009-2023.	5.8	120
99	Multiferroic decorated Fe₂O₃ monolayer predicted from first principles. Nanoscale, 2020, 12, 14847-14852.	2.8	24
100	Computational Screening of Transition Metalâ€“Phthalocyanines for the Electrochemical Reduction of Carbon Dioxide. Journal of Physical Chemistry C, 2020, 124, 7708-7715.	1.5	27
101	Polymorphism of low dimensional boron nanomaterials driven by electrostatic gating: a computational discovery. Nanoscale, 2020, 12, 10543-10549.	2.8	5
102	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. Science Bulletin, 2020, 65, 995-1002.	4.3	34
103	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
104	Edgeâ€Rich Feâˆ’N₄ Active Sites in Defective Carbon for Oxygen Reduction Catalysis. Advanced Materials, 2020, 32, e2000966.	11.1	215
105	Gradientâ€Concentration Design of Stable Coreâ€“Shell Nanostructure for Acidic Oxygen Reduction Electrocatalysis. Advanced Materials, 2020, 32, e2003493.	11.1	79
106	Water Splitting: In Situ Formation of Oxygen Vacancies Achieving Nearâ€Complete Charge Separation in Planar BiVO₄ Photoanodes (Adv. Mater. 26/2020). Advanced Materials, 2020, 32, 2070198.	11.1	3
107	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
108	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

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109	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
110	Bandstructure engineering in 2D materials using Ferroelectric materials. Applied Surface Science, 2020, 513, 145817.	3.1	9
111	Metalâ€free graphene/boron nitride heterointerface for CO₂ reduction: Surface curvature controls catalytic activity and selectivity. EcoMat, 2020, 2, e12013.	6.8	17
112	An Intrinsically Nonâ€flammable Electrolyte for Highâ€Performance Potassium Batteries. Angewandte Chemie, 2020, 132, 3667-3673.	1.6	16
113	Dimensionality-Controlled Surface Passivation for Enhancing Performance and Stability of Perovskite Solar Cells via Triethylenetetramine Vapor. ACS Applied Materials & Interfaces, 2020, 12, 6651-6661.	4.0	29
114	Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. Journal of Materials Chemistry C, 2020, 8, 7034-7040.	2.7	29
115	The effect of ethylene-amine ligands enhancing performance and stability of perovskite solar cells. Journal of Power Sources, 2020, 463, 228210.	4.0	19
116	Carbonâ€"Phosphorus Bonds-Enriched 3D Graphene by Self-Sacrificing Black Phosphorus Nanosheets for Elevating Capacitive Lithium Storage. ACS Applied Materials & Interfaces, 2020, 12, 21720-21729.	4.0	33
117	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
118	Molecular dynamic investigation of the structure and stress in crystalline and amorphous silicon during lithiation. Computational Materials Science, 2020, 183, 109811.	1.4	7
119	Reversible Intercalation of Multivalent Al 3+ Ions into Potassiumâ€Rich Cryptomelane Nanowires for Aqueous Rechargeable Alâ€Ion Batteries. ChemSusChem, 2019, 12, 3670-3670.	3.6	4
120	Ultralarge interlayer distance and C,N-codoping enable superior sodium storage capabilities of MoS2 nanoonions. Chemical Engineering Journal, 2019, 378, 122249.	6.6	39
121	Ab initio atomistic insights into lead-free formamidinium based hybrid perovskites for photovoltaics and optoelectronics. Computational Materials Science, 2019, 169, 109118.	1.4	50
122	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
123	Recent progress on the prediction of two-dimensional materials using CALYPSO. Chinese Physics B, 2019, 28, 107306.	0.7	24
124	B80 Fullerene: A Promising Metal-Free Photocatalyst for Efficient Conversion of CO2 to HCOOH. Journal of Physical Chemistry C, 2019, 123, 24193-24199.	1.5	19
125	Two-Dimensional CuTe₂X (X = Cl, Br, and I): Potential Photocatalysts for Water Splitting under the Visible/Infrared Light. Journal of Physical Chemistry C, 2019, 123, 25543-25548.	1.5	6
126	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

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127	2D boron dichalcogenides from the substitution of Mo with ionic B₂ pair in MoX₂ (X = S, Se and Te): high stability, large excitonic effect and high charge carrier mobility. Journal of Materials Chemistry C, 2019, 7, 1651-1658.	2.7	17
128	Electronic and optical properties of lead-free hybrid double perovskites for photovoltaic and optoelectronic applications. Scientific Reports, 2019, 9, 718.	1.6	130
129	Single Transition Metal Atom-Doped Graphene Supported on a Nickel Substrate: Enhanced Oxygen Reduction Reactions Modulated by Electron Coupling. Journal of Physical Chemistry C, 2019, 123, 3703-3710.	1.5	27
130	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
131	Transition metal dichalcogenides bilayer single crystals by reverse-flow chemical vapor epitaxy. Nature Communications, 2019, 10, 598.	5.8	124
132	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
133	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
134	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
135	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
136	Galvanic replacement of liquid metal galinstan with Pt for the synthesis of electrocatalytically active nanomaterials. Nanoscale, 2019, 11, 9705-9715.	2.8	43
137	Transition Metal Diborides: A New Type of Highâ€performance Electrocatalysts for Nitrogen Reduction. ChemCatChem, 2019, 11, 2624-2633.	1.8	37
138	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
139	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
140	Theoretical discovery of Dirac half metal in experimentally synthesized two dimensional metal semiquinoid frameworks. Journal of Materials Chemistry C, 2019, 7, 5792-5796.	2.7	16
141	Defective Graphene on the Transition-Metal Surface: Formation of Efficient Bifunctional Catalysts for Oxygen Evolution/Reduction Reactions in Alkaline Media. ACS Applied Materials & Interfaces, 2019, 11, 17410-17415.	4.0	34
142	Silicene catalysts for CO₂hydrogenation: the number of layers controls selectivity. Nanoscale, 2019, 11, 7734-7743.	2.8	28
143	Plasma modification of a Ni based metalâ€"organic framework for efficient hydrogen evolution. Journal of Materials Chemistry A, 2019, 7, 8129-8135.	5.2	32
144	Mo-doped boron nitride monolayer as a promising single-atom electrocatalyst for CO₂ conversion. Beilstein Journal of Nanotechnology, 2019, 10, 540-548.	1.5	34

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145	Synthesis of biphenyl bridged dendritic mesoporous organosilica with extremely high adsorption of pyrene. Journal of Materials Chemistry A, 2019, 7, 12029-12037.	5.2	25
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