Wei-jie Yang

List of Publications by Year
in descending order

81 papers	4,109 citations	117625 34 h-index	123424 61 g-index
82 all docs	82 docs citations	82 times ranked	2660 citing authors

#	Article	IF	Citations
1	A novel Fe-Co double-atom catalyst with high low-temperature activity and strong water-resistant for O3 decomposition: A theoretical exploration. Journal of Hazardous Materials, 2022, 421, 126639.	12.4	16
2	Catalytic effect of NiO/C derived from Ni-UMOFNs on the hydrogen storage performance of magnesium hydride. Journal of Alloys and Compounds, 2022, 899, 163314.	5.5	11
3	Lightâ€Assisted CO₂ Hydrogenation over Pd₃Cu@UiOâ€66 Promoted by Active Sites in Close Proximity. Angewandte Chemie - International Edition, 2022, 61, .	13.8	89
4	High throughput screening of promising lead-free inorganic halide double perovskites via first-principles calculations. Physical Chemistry Chemical Physics, 2022, 24, 3460-3469.	2.8	26
5	Density functional theory investigation of As4 adsorption on Ti, V, Cr, Mn-doped graphene. Surface Science, 2022, 720, 122049.	1.9	2
6	Exploring the Effects of Ionic Defects on the Stability of CsPbI₃ with a Deep Learning Potential. ChemPhysChem, 2022, 23, e202100841.	2.1	8
7	Simultaneous Nitrite Resourcing and Mercury Ion Removal Using MXene-Anchored Goethite Heterogeneous Fenton Composite. Environmental Science & Technology, 2022, 56, 4542-4552.	10.0	19
8	A descriptor for the structural stability of organicâ€“inorganic hybrid perovskites based on binding mechanism in electronic structure. Journal of Molecular Modeling, 2022, 28, 80.	1.8	8
9	A Sulfurâ€Tolerant MOFâ€Based Singleâ€Atom Fe Catalyst for Efficient Oxidation of NO and Hg⁰. Advanced Materials, 2022, 34, e2110123.	21.0	40
10	Direct In Situ Vertical Growth of Interlaced Mesoporous NiO Nanosheets on Carbon Felt for Electrocatalytic Ammonia Synthesis. Chemistry - A European Journal, 2022, 28, .	3.3	13
11	Linker engineering in metalâ€“organic frameworks for dark photocatalysis. Chemical Science, 2022, 13, 6696-6703.	7.4	30
12	MgH₂/single-atom heterojunctions: effective hydrogen storage materials with facile dehydrogenation. Journal of Materials Chemistry A, 2022, 10, 19839-19851.	10.3	23
13	Computational study on the adsorption of arsenic pollutants on graphene-based single-atom iron adsorbents. Physical Chemistry Chemical Physics, 2022, , .	2.8	1
14	Understanding trends in the mercury oxidation activity of single-atom catalysts. Environmental Science: Nano, 2022, 9, 2041-2050.	4.3	13
15	Small practical cluster models for perovskites based on the similarity criterion of central location environment and their applications. Physical Chemistry Chemical Physics, 2022, 24, 14375-14389.	2.8	6
16	Microwave-Induced Deep Catalytic Oxidation of NO Using Molecular-Sieve-Supported Oxygen-Vacancy-Enriched Feâ€“Mn Bimetal Oxides. Environmental Science & Technology, 2022, 56, 10423-10432.	10.0	11
17	Reaction Behavior and Cost-Effectiveness of Halogen Radicals in Hg⁰ Removal: Performance, Kinetics, and Mechanism. ACS ES&T Engineering, 2021, 1, 66-75.	7.6	6
18	Integration of Pd nanoparticles with engineered pore walls in MOFs for enhanced catalysis. CheM, 2021, 7, 686-698.	11.7	146

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19	A new perspective for evaluating the photoelectric performance of organicâ€“inorganic hybrid perovskites based on the DFT calculations of excited states. Physical Chemistry Chemical Physics, 2021, 23, 11548-11556.	2.8	23
20	Origin of the hydrophobicity of sulfur-containing iron surfaces. Physical Chemistry Chemical Physics, 2021, 23, 13971-13976.	2.8	38
21	Rational Fabrication of Lowâ€Coordinate Singleâ€Atom Ni Electrocatalysts by MOFs for Highly Selective CO₂ Reduction. Angewandte Chemie - International Edition, 2021, 60, 7607-7611.	13.8	368
22	Rational Fabrication of Lowâ€Coordinate Singleâ€Atom Ni Electrocatalysts by MOFs for Highly Selective CO₂ Reduction. Angewandte Chemie, 2021, 133, 7685-7689.	2.0	39
23	Modulating Coordination Environment of Single-Atom Catalysts and Their Proximity to Photosensitive Units for Boosting MOF Photocatalysis. Journal of the American Chemical Society, 2021, 143, 12220-12229.	13.7	219
24	Nanozyme with Robust Catalase Activity by Multiple Mechanisms and Its Application for Hypoxic Tumor Treatment. Advanced Healthcare Materials, 2021, 10, e2100601.	7.6	35
25	Density functional theory investigation of As4, As2 and AsH3 adsorption on Ti-doped graphene. Chemical Engineering Journal, 2021, 421, 129747.	12.7	12
26	Single-atom iron as a promising low-temperature catalyst for selective catalytic reduction of NO with NH3: A theoretical prediction. Fuel, 2021, 302, 121041.	6.4	36
27	Construction of transition metal-decorated boron doped twin-graphene for hydrogen storage: A theoretical prediction. Fuel, 2021, 304, 121351.	6.4	50
28	Design of (C3N2H5)(1-)Cs PbI3 as a novel hybrid perovskite with strong stability and excellent photoelectric performance: A theoretical prediction. Solar Energy Materials and Solar Cells, 2021, 233, 111401.	6.2	7
29	CO2 adsorption and dissociation on single and double iron atomic molybdenum disulfide catalysts: A DFT study. Fuel, 2021, 305, 121547.	6.4	16
30	Screening for lead-free inorganic double perovskites with suitable band gaps and high stability using combined machine learning and DFT calculation. Applied Surface Science, 2021, 568, 150916.	6.1	38
31	Screening MXenes for novel anode material of lithium-ion batteries with high capacity and stability: A DFT calculation. Applied Surface Science, 2021, 569, 151050.	6.1	48
32	Methane activation on dual-atom catalysts supported on graphene. Chemical Communications, 2021, 57, 12127-12130.	4.1	6
33	First-Principles Study on the Stability and Electronic Properties of Dionâ€“Jacobson Halide Aâ€²(MA)_{nâ^'1}B_nX_{3n+1} Perovskites. Journal of Physical Chemistry C, 2021, 125, 24096-24104.	3.1	14
34	A First-Principles Study on Titanium-Decorated Adsorbent for Hydrogen Storage. Energies, 2021, 14, 6845.	3.1	10
35	Non-Bonding Interaction of Neighboring Fe and Ni Single-Atom Pairs on MOF-Derived N-Doped Carbon for Enhanced CO₂ Electroreduction. Journal of the American Chemical Society, 2021, 143, 19417-19424.	13.7	305
36	LiBH4 for hydrogen storage - New perspectives. Nano Materials Science, 2020, 2, 109-119.	8.8	41

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37	Geometric structures, electronic characteristics, stabilities, catalytic activities, and descriptors of graphene-based single-atom catalysts. Nano Materials Science, 2020, 2, 120-131.	8.8	55
38	Theoretical prediction of graphene-based single-atom iron as a novel catalyst for catalytic oxidation of Hg0 by O2. Applied Surface Science, 2020, 508, 145035.	6.1	27
39	Theoretical study on double-atom catalysts supported with graphene for electroreduction of nitrogen into ammonia. Electrochimica Acta, 2020, 335, 135667.	5.2	62
40	Mechanism study on CO2 reforming of methane over platinum cluster doped graphene: A DFT calculation. Molecular Catalysis, 2020, 497, 111205.	2.0	8
41	Catalytic oxidation degradation of formaldehyde on FeN3-graphene surface: A DFT study. Applied Surface Science, 2020, 534, 147594.	6.1	21
42	Singleâ€Atom Electrocatalysts from Multivariate Metalâ€“Organic Frameworks for Highly Selective Reduction of CO₂ at Low Pressures. Angewandte Chemie - International Edition, 2020, 59, 20589-20595.	13.8	247
43	Metalâ€“Organic Frameworks: Boosting Catalysis of Pd Nanoparticles in MOFs by Pore Wall Engineering: The Roles of Electron Transfer and Adsorption Energy (Adv. Mater. 30/2020). Advanced Materials, 2020, 32, 2070225.	21.0	24
44	Singleâ€Atom Electrocatalysts from Multivariate Metalâ€“Organic Frameworks for Highly Selective Reduction of CO₂ at Low Pressures. Angewandte Chemie, 2020, 132, 20770-20776.	2.0	37
45	Computational design of (100) alloy surfaces for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2020, 8, 17987-17997.	10.3	47
46	A comprehensive exploration of mercury adsorption sites on the carbonaceous surface: A DFT study. Fuel, 2020, 282, 118781.	6.4	34
47	Mechanism of hydrogen storage on Fe₃B. Chemical Communications, 2020, 56, 14235-14238.	4.1	13
48	Screening the activity of single-atom catalysts for the catalytic oxidation of sulfur dioxide with a kinetic activity model. Chemical Communications, 2020, 56, 11657-11660.	4.1	12
49	Accelerating Chemo- and Regioselective Hydrogenation of Alkynes over Bimetallic Nanoparticles in a Metalâ€“Organic Framework. ACS Catalysis, 2020, 10, 7753-7762.	11.2	80
50	Identifying the active sites of carbonaceous surface for the adsorption of gaseous arsenic trioxide: A theoretical study. Chemical Engineering Journal, 2020, 402, 125800.	12.7	34
51	Nanocasting SiO2 into metalâ€“organic frameworks imparts dual protection to high-loading Fe single-atom electrocatalysts. Nature Communications, 2020, 11, 2831.	12.8	321
52	Boosting Catalysis of Pd Nanoparticles in MOFs by Pore Wall Engineering: The Roles of Electron Transfer and Adsorption Energy. Advanced Materials, 2020, 32, e2000041.	21.0	151
53	On the adsorption of elemental mercury on single-atom TM (TMÂ=ÂV, Cr, Mn, Co) decorated graphene substrates. Applied Surface Science, 2020, 516, 146037.	6.1	17
54	Regulating the coordination environment through doping N atoms for single-atom Mn electrocatalyst of N2 reduction with high catalytic activity and selectivity: A theoretical study. Molecular Catalysis, 2020, 493, 111091.	2.0	15

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55	The effect of coordination environment on the kinetic and thermodynamic stability of single-atom iron catalysts. Physical Chemistry Chemical Physics, 2020, 22, 3983-3989.	2.8	45
56	CO2 hydrogenation to formic acid over platinum cluster doped defective graphene: A DFT study. Applied Surface Science, 2020, 517, 146200.	6.1	27
57	Simultaneous catalytic oxidation of nitric oxide and elemental mercury by single-atom Pd/g-C3N4 catalyst: A DFT study. Molecular Catalysis, 2020, 488, 110901.	2.0	16
58	Adsorption behavior of Pt embedded on Nâ€doped graphene sheets toward NO and NH₃ molecules. Applied Organometallic Chemistry, 2019, 33, e5079.	3.5	14
59	Car-Parrinello molecular dynamics study on the interaction between lignite and water molecules. Fuel, 2019, 258, 116189.	6.4	19
60	Hg0 oxidation and SO3, Pb0, PbO, PbCl2 and As2O3 adsorption by graphene-based bimetallic catalyst ((Fe,Co)@N-GN): A DFT study. Applied Surface Science, 2019, 496, 143686.	6.1	38
61	Theoretical insights into the stability of perovskite clusters by studying water adsorption on (CH3NH3)4SnI6. Solar Energy Materials and Solar Cells, 2019, 202, 110126.	6.2	3
62	The adsorption and activation of oxygen molecule on nickel clusters doped graphene-based support by DFT. Molecular Catalysis, 2019, 477, 110547.	2.0	12
63	Directly catalytic reduction of NO without NH3 by single atom iron catalyst: A DFT calculation. Fuel, 2019, 243, 262-270.	6.4	94
64	Adsorption behavior of mercuric oxide clusters on activated carbon and the effect of SO2 on this adsorption: a theoretical investigation. Journal of Molecular Modeling, 2019, 25, 142.	1.8	18
65	Density functional study of the adsorption of NO on Ni (nâ€¯=â€¯1, 2, 3 and 4) clusters doped functionalized graphene support. Applied Surface Science, 2019, 481, 940-950.	6.1	27
66	Adsorption characteristics of Co-anchored different graphene substrates toward O2 and NO molecules. Applied Surface Science, 2019, 480, 779-791.	6.1	29
67	Bimetallic sites supported on N-doped graphene ((Fe,Co)/N-GN) as a new catalyst for NO oxidation: A theoretical investigation. Molecular Catalysis, 2019, 470, 56-66.	2.0	33
68	Single-atom catalysts templated by metalâ€“organic frameworks for electrochemical nitrogen reduction. Journal of Materials Chemistry A, 2019, 7, 26371-26377.	10.3	152
69	The adsorption characteristics of As2O3, Pb0, PbO and PbCl2 on single atom iron adsorbent with graphene-based substrates. Chemical Engineering Journal, 2019, 361, 304-313.	12.7	77
70	Weak interaction between water molecule and different rank coals: a DFT-D3 study. International Journal of Oil, Gas and Coal Technology, 2019, 21, 91.	0.2	0
71	Support effects on adsorption and catalytic activation of O₂ in single atom iron catalysts with graphene-based substrates. Physical Chemistry Chemical Physics, 2018, 20, 7333-7341.	2.8	64
72	Support effects in single atom iron catalysts on adsorption characteristics of toxic gases (NO2, NH3,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	6.1	81

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73	Single-atom iron catalyst with single-vacancy graphene-based substrate as a novel catalyst for NO oxidation: a theoretical study. Catalysis Science and Technology, 2018, 8, 4159-4168.	4.1	76
74	Effects of oxygen functional complexes on arsenic adsorption over carbonaceous surface. Journal of Hazardous Materials, 2018, 360, 436-444.	12.4	66
75	Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO) Tj ETQq1 1 0.784314 rgBT /Over	6.1	58
76	The adsorption characteristics of mercury species on single atom iron catalysts with different graphene-based substrates. Applied Surface Science, 2018, 455, 940-951.	6.1	50
77	DFT study of water adsorption on lignite molecule surface. Journal of Molecular Modeling, 2017, 23, 27.	1.8	30
78	Theoretical research on heterogeneous reduction of N2O by char. Applied Thermal Engineering, 2017, 126, 28-36.	6.0	61
79	Effects of CO/CO2/NO on elemental lead adsorption on carbonaceous surfaces. Journal of Molecular Modeling, 2016, 22, 166.	1.8	20
80	Quantum chemistry investigation on the reaction mechanism of the elemental mercury, chlorine, bromine and ozone system. Journal of Molecular Modeling, 2015, 21, 160.	1.8	10
81	Lightâ€Assisted CO 2 Hydrogenation over Pd 3 Cu@UiOâ€66 Promoted by Active Sites in Close Proximity. Angewandte Chemie, 0, , .	2.0	11