Dongwei

List of Publications by Year
in descending order

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96 papers	5,591 citations	50566 48 h-index	90395 73 g-index
96 all docs	96 docs citations	96 times ranked	5259 citing authors

#	Article	IF	Citations
1	Surface Van Hove Singularity Enabled Efficient Catalysis in Low-Dimensional Systems: CO Oxidation and Hydrogen Evolution Reactions. Journal of Physical Chemistry Letters, 2022, 13, 740-746.	2.1	10
2	Electrocatalytic two-electron oxygen reduction over nitrogen doped hollow carbon nanospheres. Chemical Communications, 2022, 58, 5025-5028.	2.2	14
3	An efficient screening strategy towards multifunctional catalysts for the simultaneous electroreduction of NO₃^â, NO₂^â and NO to NH₃. Journal of Materials Chemistry A, 2022, 10, 9707-9716.	5.2	52
4	Coupling denitrification and ammonia synthesis via selective electrochemical reduction of nitric oxide over Fe₂O₃ nanorods. Journal of Materials Chemistry A, 2022, 10, 6454-6462.	5.2	52
5	Conductive Two-Dimensional Magnesium Metalâ€“Organic Frameworks for High-Efficiency O₂ Electroreduction to H₂O₂. ACS Catalysis, 2022, 12, 6092-6099.	5.5	78
6	Theoretical insights into the electroreduction of nitrate to ammonia on graphene-based single-atom catalysts. Nanoscale, 2022, 14, 10862-10872.	2.8	57
7	Theoretical screening of the transition metal heteronuclear dimer anchored graphdiyne for electrocatalytic nitrogen reduction. Journal of Energy Chemistry, 2021, 54, 501-509.	7.1	116
8	A magnetron sputtered Mo₃Si thin film: an efficient electrocatalyst for N₂ reduction under ambient conditions. Journal of Materials Chemistry A, 2021, 9, 884-888.	5.2	72
9	Enabling multifunctional electrocatalysts by modifying the basal plane of unifunctional 1Tâ€²-MoS₂ with anchored transition metal single atoms. Nanoscale, 2021, 13, 13390-13400.	2.8	69
10	Electrocatalytic nitrogen reduction on the transition-metal dimer anchored N-doped graphene: performance prediction and synergetic effect. Physical Chemistry Chemical Physics, 2021, 23, 4018-4029.	1.3	90
11	Single-atom catalysts based on TiN for the electrocatalytic hydrogen evolution reaction: a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 15685-15692.	1.3	6
12	Enhanced Electrochemical H₂O₂ Production via Two-Electron Oxygen Reduction Enabled by Surface-Derived Amorphous Oxygen-Deficient TiO_{2â€“x}. ACS Applied Materials & Interfaces, 2021, 13, 33182-33187.	4.0	67
13	Optimizing the Electronic Structure of ZnS via Cobalt Surface Doping for Promoted Photocatalytic Hydrogen Production. Inorganic Chemistry, 2021, 60, 15712-15723.	1.9	14
14	High-efficiency electrochemical nitrite reduction to ammonium using a Cu₃P nanowire array under ambient conditions. Green Chemistry, 2021, 23, 5487-5493.	4.6	73
15	Boron-decorated C₉N₄ monolayers as promising metal-free catalysts for electrocatalytic nitrogen reduction reaction: a first-principles study. New Journal of Chemistry, 2020, 44, 422-427.	1.4	34
16	Enhanced electrocatalytic N₂-to-NH₃ fixation by ZrS₂ nanofibers with a sulfur vacancy. Chemical Communications, 2020, 56, 14031-14034.	2.2	25
17	Ambient electrochemical NH₃ synthesis from N₂ and water enabled by ZrO₂ nanoparticles. Chemical Communications, 2020, 56, 3673-3676.	2.2	59
18	Porous LaFeO3 nanofiber with oxygen vacancies as an efficient electrocatalyst for N2 conversion to NH3 under ambient conditions. Journal of Energy Chemistry, 2020, 50, 402-408.	7.1	87

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19	Computational Evaluation of Electrocatalytic Nitrogen Reduction on TM Single-, Double-, and Triple-Atom Catalysts (TM = Mn, Fe, Co, Ni) Based on Graphdiyne Monolayers. Journal of Physical Chemistry C, 2019, 123, 19066-19076.	1.5	224
20	Boron-doped InSe monolayer as a promising electrocatalyst for nitrogen reduction into ammonia at ambient conditions. Applied Surface Science, 2019, 495, 143463.	3.1	46
21	Transition metal embedded C₃N monolayers as promising catalysts for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2019, 21, 20432-20441.	1.3	32
22	Metal- and Nonmetal-Atom-Modified Graphene as Efficient Catalysts for CO Oxidation Reactions. Journal of Physical Chemistry C, 2019, 123, 10926-10939.	1.5	28
23	A first-principles study of doped black phosphorus carbide monolayers as NO2 and NH3 sensors. Journal of Applied Physics, 2019, 125, .	1.1	17
24	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. Applied Surface Science, 2019, 479, 590-594.	3.1	26
25	Repairing single and double atomic vacancies in a C₃N monolayer with CO or NO molecules: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 13517-13527.	1.3	41
26	A computational study of CO oxidation reactions on metal impurities in graphene divacancies. Physical Chemistry Chemical Physics, 2018, 20, 2284-2295.	1.3	52
27	Detection of gas molecules on single Mn adatom adsorbed graphyne: a DFT-D study. Journal Physics D: Applied Physics, 2018, 51, 065109.	1.3	56
28	First-principles study on the gas sensing property of the Ge, As, and Br doped PtSe₂. Materials Research Express, 2018, 5, 035037.	0.8	13
29	The role of the intrinsic Se and In vacancies in the interaction of O2 and H2O molecules with the InSe monolayer. Applied Surface Science, 2018, 434, 215-227.	3.1	27
30	First-Principles Study on the Single Ir Atom Embedded Graphdiyne: An Efficient Catalyst for CO Oxidation. Journal of Physical Chemistry C, 2018, 122, 23481-23492.	1.5	87
31	Boron-Doped C₃N Monolayer as a Promising Metal-Free Oxygen Reduction Reaction Catalyst: A Theoretical Insight. Journal of Physical Chemistry C, 2018, 122, 20312-20322.	1.5	78
32	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. Carbon, 2017, 118, 35-42.	5.4	164
33	Mechanisms of direct hydrogen peroxide synthesis on silicon and phosphorus dual-doped graphene: a DFT-D study. Physical Chemistry Chemical Physics, 2017, 19, 9007-9015.	1.3	18
34	Sulfur doped graphene as a promising metal-free electrocatalyst for oxygen reduction reaction: a DFT-D study. RSC Advances, 2017, 7, 20398-20405.	1.7	53
35	Interaction between H₂O, N₂, CO, NO, NO₂ and N₂O molecules and a defective WSe₂ monolayer. Physical Chemistry Chemical Physics, 2017, 19, 26022-26033.	1.3	60
36	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. Applied Surface Science, 2017, 426, 1232-1240.	3.1	99

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37	Tuning the Physical and Chemical Properties of 2D InSe with Interstitial Boron Doping: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 28312-28316.	1.5	11
38	Au cluster adsorption on perfect and defective MoS₂ monolayers: structural and electronic properties. Physical Chemistry Chemical Physics, 2017, 19, 20735-20748.	1.3	103
39	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. Applied Surface Science, 2017, 394, 47-57.	3.1	11
40	Adsorption sensitivity of metal atom decorated bilayer graphene toward toxic gas molecules (CO, NO,) Tj ETQq0 0 0 rgBT /Overlock 10 T	4.0	105
41	Surface-dominated negative photoresponse of phosphorus-doped ZnSe nanowires and their detecting performance. Journal of Materials Science: Materials in Electronics, 2016, 27, 11463-11469.	1.1	9
42	CO oxidation catalyzed by the single Co atom embedded hexagonal boron nitride nanosheet: a DFT-D study. Physical Chemistry Chemical Physics, 2016, 18, 21865-21870.	1.3	96
43	The atomic structures and electronic properties of potassium-doped phenanthrene from a first-principles study. Journal of Materials Chemistry C, 2016, 4, 11566-11571.	2.7	11
44	Electronic structure and high thermoelectric properties of a new material Ba3Cu20Te13. Journal of Alloys and Compounds, 2016, 678, 12-17.	2.8	7
45	The unexpectedly rich reconstructions of rutile TiO2(011)-(2 Ã— 1) surface and the driving forces behind their formation: an ab initio evolutionary study. Physical Chemistry Chemical Physics, 2016, 18, 19549-19556.	1.3	18
46	Formaldehyde molecule adsorption on the doped monolayer MoS2: A first-principles study. Applied Surface Science, 2016, 371, 180-188.	3.1	129
47	3d transition metal embedded C2N monolayers as promising single-atom catalysts: A first-principles study. Carbon, 2016, 105, 463-473.	5.4	167
48	The adsorption of CO and NO on the MoS2 monolayer doped with Au, Pt, Pd, or Ni: A first-principles study. Applied Surface Science, 2016, 383, 98-105.	3.1	321
49	The mechanism of oxygen activation on single Pt-atom doped SnO2(110) surface. Journal of Materials Science, 2016, 51, 10400-10407.	1.7	32
50	Magnetic and Electronic Properties of Samarium-Doped Phenanthrene from First-Principles Study. Journal of Physical Chemistry C, 2016, 120, 22565-22570.	1.5	12
51	Tuning metal cluster catalytic activity with morphology and composition: a DFT study of O₂ dissociation at the global minimum of Pt_mPd_n (m + n = 5) clusters. RSC Advances, 2016, 6, 104388-104397.	1.7	19
52	Repairing sulfur vacancies in the MoS₂ monolayer by using CO, NO and NO₂ molecules. Journal of Materials Chemistry C, 2016, 4, 7093-7101.	2.7	111
53	Catalytic conversion of CHx and CO2 on non-noble metallic impurities in graphene. Physical Chemistry Chemical Physics, 2016, 18, 16998-17009.	1.3	6
54	Insight into the mechanism of Pt anchored graphene toward the CHx(xÂ=Â1Ââ¼Â4) reforming under H2 environments. International Journal of Hydrogen Energy, 2016, 41, 13197-13207.	3.8	5

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55	First principles study on the interfacial properties of NM/graphdiyne (NM = Pd, Pt, Rh and Ir): The implications for NM growing. Applied Surface Science, 2016, 360, 1-7.	3.1	90
56	Modulating electronic, magnetic and chemical properties of MoS2 monolayer sheets by substitutional doping with transition metals. Applied Surface Science, 2016, 364, 181-189.	3.1	161
57	First-principles study of O2 adsorption on Al-doped ZnO(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 682 Td (xmlns:mml=	4.0	25
58	surface. Sensors and Actuators B: Chemical, 2016, 224, 372-380. Novel catalytic activity for oxygen reduction reaction on MnN4 embedded graphene: A dispersion-corrected density functional theory study. Carbon, 2015, 84, 500-508.	5.4	166
59	Improving the adsorption behavior and reaction activity of Co-anchored graphene surface toward CO and O2 molecules. Sensors and Actuators B: Chemical, 2015, 211, 227-234.	4.0	63
60	Coadsorption of gold with chlorine on CeO ₂ (111) surfaces: A first principles study. Chinese Physics B, 2015, 24, 026801.	0.7	3
61	Adsorption and oxidation of NO on various SnO2(1 1 0) surfaces: A density functional theory study. Sensors and Actuators B: Chemical, 2015, 221, 717-722.	4.0	51
62	Dependence of memory characteristics on the (ZrO₂)_x(SiO₂)_{1â^'x}elemental composition for charge trap flash memory applications. Semiconductor Science and Technology, 2015, 30, 065010.	1.0	8
63	Single Pt atom stabilized on nitrogen doped graphene: CO oxidation readily occurs via the tri-molecular Eleyâ€“Rideal mechanism. Physical Chemistry Chemical Physics, 2015, 17, 20006-20013.	1.3	91
64	Adsorption behavior of Co anchored on graphene sheets toward NO, SO2, NH3, CO and HCN molecules. Applied Surface Science, 2015, 342, 191-199.	3.1	132
65	Pd₁/BN as a promising single atom catalyst of CO oxidation: a dispersion-corrected density functional theory study. RSC Advances, 2015, 5, 84381-84388.	1.7	68
66	Construction of ZnSeâ€“ZnO axial pâ€“n junctions via regioselective oxidation process and their photo-detection applications. Applied Surface Science, 2015, 357, 1939-1943.	3.1	10
67	Graphyne as a promising substrate for the noble-metal single-atom catalysts. Carbon, 2015, 95, 756-765.	5.4	181
68	CO catalytic oxidation on Al-doped graphene-like ZnO monolayer sheets: a first-principles study. Journal of Materials Chemistry C, 2015, 3, 9964-9972.	2.7	58
69	Adsorption and dissociation of ammonia on small iron clusters. International Journal of Hydrogen Energy, 2015, 40, 346-352.	3.8	23
70	CO catalytic oxidation on iron-embedded monolayer MoS2. Applied Surface Science, 2015, 328, 71-77.	3.1	100
71	The mechanisms of oxygen reduction reaction on phosphorus doped graphene: A first-principles study. Journal of Power Sources, 2015, 276, 222-229.	4.0	165
72	The elastic and thermoelectric properties of the Zintl compound Ca5Al2Sb6 under high pressure. Journal of Applied Physics, 2014, 116, .	1.1	10

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73	O2 activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. Applied Surface Science, 2014, 300, 91-97.	3.1	11
74	Depletion NO x Made Easy by Nitrogen Doped Graphene. Catalysis Letters, 2014, 144, 1016-1022.	1.4	16
75	Ag (100)/MgO (100) interface: A van der Waals density functional study. Applied Surface Science, 2014, 288, 115-121.	3.1	7
76	Formation and catalytic activity of Pt supported on oxidized graphene for the CO oxidation reaction. Physical Chemistry Chemical Physics, 2014, 16, 7887-7895.	1.3	75
77	A density function theory study on the NO reduction on nitrogen doped graphene. Physical Chemistry Chemical Physics, 2014, 16, 20561-20569.	1.3	53
78	Effect of lattice strain on the oxygen vacancy formation and hydrogen adsorption at CeO2(111) surface. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2570-2575.	0.9	82
79	Direct CO oxidation by lattice oxygen on the SnO₂(110) surface: a DFT study. Physical Chemistry Chemical Physics, 2014, 16, 12488-12494.	1.3	51
80	Adsorption and oxidation of sulfur dioxide on the yttria-stabilized zirconia surface: ab initio atomistic thermodynamics study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 659-666.	0.9	5
81	Theoretical study on the Si-doped graphene as an efficient metal-free catalyst for CO oxidation. Applied Surface Science, 2014, 308, 402-407.	3.1	115
82	Tuning the catalytic property of non-noble metallic impurities in graphene. Carbon, 2014, 71, 139-149.	5.4	85
83	The sulfur tolerance mechanism of the Cu/CeO2 system. International Journal of Hydrogen Energy, 2014, 39, 1957-1966.	3.8	5
84	Effects of Composition on the Memory Characteristics of (HfO2)x(Al2O3)1-xBased Charge Trap Nonvolatile Memory. Transactions on Electrical and Electronic Materials, 2014, 15, 241-244.	1.0	1
85	Dependence of Electrons Loss Behavior on the Nitride Thickness and Temperature for Charge Trap Flash Memory Applications. Transactions on Electrical and Electronic Materials, 2014, 15, 245-248.	1.0	0
86	First-principles studies of Fe atoms adsorption on hydrogen-terminated boron nitride nanoribbons. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 1016-1020.	0.9	14
87	Formation, Stabilities, and Electronic and Catalytic Performance of Platinum Catalyst Supported on Non-Metal-Doped Graphene. Journal of Physical Chemistry C, 2013, 117, 5258-5268.	1.5	78
88	First-principles studies of BN sheets with absorbed transition metal single atoms or dimers: stabilities, electronic structures, and magnetic properties. Journal of Physics Condensed Matter, 2012, 24, 145501.	0.7	33
89	First principles study of the magnetism driven by cation defects in CeO₂: the important role of O2p states. Chinese Physics B, 2012, 21, 047505.	0.7	8
90	Strong spinâ€“orbit splitting in graphene with adsorbed Au atoms. Carbon, 2012, 50, 297-305.	5.4	76

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91	Origin of the High Activity of the Ceria-Supported Copper Catalyst for H₂O Dissociation. Journal of Physical Chemistry C, 2011, 115, 6730-6740.	1.5	52
92	First-principles studies of Pb doping in graphene: stability, energy gap and spinâ€“orbit splitting. New Journal of Physics, 2011, 13, 123018.	1.2	23
93	The main factors influencing the O vacancy formation on the Ir doped ceria surface: A DFT+U study. European Physical Journal B, 2010, 77, 373-380.	0.6	20
94	The Effect of Environment on the Reaction of Water on the Ceria(111) Surface: A DFT+U Study. Journal of Physical Chemistry C, 2010, 114, 14891-14899.	1.5	105
95	The properties of the Pt6/BaO(100) interface and NO adsorption at the interface. Surface Science, 2009, 603, 2413-2421.	0.8	1
96	Designing Multifunctional Donorâ€“Acceptor-Type Molecules to Passivate Surface Defects Efficiently and Enhance Charge Transfer of CsPbI₂Br Perovskite for High Power Conversion Efficiency. Inorganic Chemistry, 0, , .	1.9	1