Zongxian Yang

List of Publications by Year
in descending order

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212 papers	7,872 citations	43973 48 h-index	64668 79 g-index
212 all docs	212 docs citations	212 times ranked	7024 citing authors

#	Article	IF	Citations
1	Atomic and electronic structure of unreduced and reduced CeO2 surfaces: A first-principles study. Journal of Chemical Physics, 2004, 120, 7741-7749.	1.2	338
2	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
3	A theoretical simulation on the catalytic oxidation of CO on Pt/graphene. Physical Chemistry Chemical Physics, 2012, 14, 16566.	1.3	297
4	Bifunctional CoNx embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. Carbon, 2018, 130, 112-119.	5.4	209
5	C3N monolayers as promising candidates for NO2 sensors. Sensors and Actuators B: Chemical, 2018, 266, 664-673.	4.0	172
6	3d transition metal embedded C2N monolayers as promising single-atom catalysts: A first-principles study. Carbon, 2016, 105, 463-473.	5.4	167
7	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
8	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
9	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. Carbon, 2017, 118, 35-42.	5.4	164
10	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
11	Effects of Zr doping on stoichiometric and reduced ceria: A first-principles study. Journal of Chemical Physics, 2006, 124, 224704.	1.2	131
12	Formaldehyde molecule adsorption on the doped monolayer MoS2: A first-principles study. Applied Surface Science, 2016, 371, 180-188.	3.1	129
13	Theoretical Inspection of M₁/PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). ACS Catalysis, 2021, 11, 8929-8941.	5.5	121
14	Trapping of metal atoms in the defects on graphene. Journal of Chemical Physics, 2011, 135, 224704.	1.2	116
15	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
16	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
17	Physisorbed, Chemisorbed, and Oxidized CO on Highly Active Cuâ"CeO₂(111). Journal of Physical Chemistry C, 2010, 114, 4486-4494.	1.5	110
18	Strong and weak adsorption of CO on CeO2 surfaces from first principles calculations. Chemical Physics Letters, 2004, 396, 384-392.	1.2	108

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19	Oxygen vacancy formation energy in Pd-doped ceria: A DFT+U study. Journal of Chemical Physics, 2007, 127, 074704.	1.2	105
20	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
21	A promising single atom catalyst for CO oxidation: Ag on boron vacancies of h-BN sheets. Physical Chemistry Chemical Physics, 2017, 19, 16795-16805.	1.3	102
22	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. Applied Surface Science, 2017, 426, 1232-1240.	3.1	99
23	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
24	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
25	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
26	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
27	Tuning the catalytic property of non-noble metallic impurities in graphene. Carbon, 2014, 71, 139-149.	5.4	85
28	First-principles study of thePtâˆ•CeO2(111)interface. Physical Review B, 2007, 76, .	1.1	82
29	Single Pd atomic catalyst on Mo₂CO₂ monolayer (MXene): unusual activity for CO oxidation by trimolecular Eleyâ€“Rideal mechanism. Physical Chemistry Chemical Physics, 2018, 20, 3504-3513.	1.3	82
30	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
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	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
33	Oxygen vacancy formation energy at the Pd/CeO2(111) interface. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 369, 132-139.	0.9	70
34	Facile synthesis of hollow palladium/copper alloyed nanocubes for formic acid oxidation. Chemical Communications, 2011, 47, 8581.	2.2	70
35	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. Surface Science, 2008, 602, 1199-1206.	0.8	68
36	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

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37	Single non-noble-metal cobalt atom stabilized by pyridinic vacancy graphene: An efficient catalyst for CO oxidation. Journal of Molecular Catalysis A, 2016, 417, 28-35.	4.8	68
38	3D well-ordered porous phosphorus doped carbon as an anode for sodium storage: structure design, experimental and computational insights. Journal of Materials Chemistry A, 2019, 7, 11400-11407.	5.2	64
39	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
40	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
41	The sensing mechanism of Pt-doped SnO2 surface toward CO: A first-principle study. Sensors and Actuators B: Chemical, 2014, 202, 83-92.	4.0	55
42	Cu-doped ceria: Oxygen vacancy formation made easy. Chemical Physics Letters, 2011, 510, 60-66.	1.2	53
43	A density function theory study on the NO reduction on nitrogen doped graphene. Physical Chemistry Chemical Physics, 2014, 16, 20561-20569.	1.3	53
44	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
45	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
46	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
47	The mechanism of oxygen reduction reaction on CoN4 embedded graphene: A combined kinetic and atomistic thermodynamic study. International Journal of Hydrogen Energy, 2016, 41, 21212-21220.	3.8	51
48	Cu₃-Cluster-Doped Monolayer Mo₂CO₂ (MXene) as an Electron Reservoir for Catalyzing a CO Oxidation Reaction. ACS Applied Materials & Interfaces, 2018, 10, 32903-32912.	4.0	51
49	First-principles study of the adsorption of sulfur on Pt(111): S core-level shifts and the nature of the Pt-S bond. Physical Review B, 2002, 65, .	1.1	48
50	CO2 thermoreduction to methanol on the MoS2 supported single Co atom catalyst: A DFT study. Applied Surface Science, 2020, 528, 147047.	3.1	46
51	Oxygen vacancy pairs on CeO2(110): A DFT+U study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2786-2792.	0.9	44
52	Noble metals induced magnetic properties of graphene. Journal of Magnetism and Magnetic Materials, 2011, 323, 2441-2447.	1.0	44
53	Tunable magnetic and electronic properties of the Cr-based MXene (Cr2C) with functional groups and doping. Journal of Magnetism and Magnetic Materials, 2020, 514, 167141.	1.0	42
54	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

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55	Structural and electronic properties of NM-doped ceria (NM = Pt, Rh): a first-principles study. Journal of Physics Condensed Matter, 2008, 20, 035210.	0.7	39
56	Direct CO Oxidation by Lattice Oxygen on Zr-Doped Ceria Surfaces. Catalysis Letters, 2011, 141, 78-82.	1.4	39
57	Tailoring the Electronic Structure of Transition Metals by the V₂C MXene Support: Excellent Oxygen Reduction Performance Triggered by Metalâ€“Support Interactions. ACS Applied Materials & Interfaces, 2020, 12, 28206-28216.	4.0	39
58	The adsorption, diffusion and dissociation of O2 on Pt-skin Pt3Ni(111): A density functional theory study. Chemical Physics Letters, 2010, 499, 83-88.	1.2	38
59	Interfacial properties of NM/CeO₂(111) (NM = noble metal atoms or clusters of Pd, Pt and) Tj ETQq1 1 0.784314 rgBT /Ov	0.7	34
60	Preventing the CO poisoning on Pt nanocatalyst using appropriate substrate: a first-principles study. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	34
61	A comparison study of oxygen reduction on the supported Pt, Pd, Au monolayer on WC(0001). Journal of Power Sources, 2016, 321, 163-173.	4.0	34
62	Electronic structure and optical properties for blue phosphorene/graphene-like GaN van der Waals heterostructures. Current Applied Physics, 2017, 17, 1714-1720.	1.1	34
63	SOx on ceria from adsorbed SO2. Journal of Chemical Physics, 2011, 134, 184703.	1.2	32
64	The mechanism of oxygen activation on single Pt-atom doped SnO2(110) surface. Journal of Materials Science, 2016, 51, 10400-10407.	1.7	32
65	Recent progress of MXenes as the support of catalysts for the CO oxidation and oxygen reduction reaction. Chinese Chemical Letters, 2020, 31, 931-936.	4.8	32
66	Cr2NX2 MXene (X = O, F, OH): A 2D ferromagnetic half-metal. Applied Physics Letters, 2021, 119, .	1.5	32
67	Density functional theory studies on the adsorption, diffusion and dissociation of O2 on Pt(111). Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 4713-4717.	0.9	31
68	The synergistic effects of the Cuâ€“CeO2(111) catalysts on the adsorption and dissociation of water molecules. Physical Chemistry Chemical Physics, 2011, 13, 9363.	1.3	31
69	Additive-Free Fabrication of Spherical Hollow Palladium/Copper Alloyed Nanostructures for Fuel Cell Application. ACS Applied Materials & Interfaces, 2012, 4, 4461-4464.	4.0	31
70	Tuning the ORR activity of Pt-based Ti₂CO₂ MXenes by varying the atomic cluster size and doping with metals. Nanoscale, 2020, 12, 12497-12507.	2.8	31
71	Identification of Efficient Single-Atom Catalysts Based on V₂CO₂ MXene by ab Initio Simulations. Journal of Physical Chemistry C, 2020, 124, 4090-4100.	1.5	31
72	Density Functional Theory Study of Sn Adsorption on the CeO₂Surface. Journal of Physical Chemistry C, 2011, 115, 16461-16466.	1.5	30

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73	Novel two-dimensional ferroelectric PbTe under tension: A first-principles prediction. Journal of Applied Physics, 2017, 122, .	1.1	30
74	Effects of rare-earth doping on the ionic conduction of CeO2 in solid oxide fuel cells. Ceramics International, 2018, 44, 3707-3711.	2.3	30
75	Engineering the activity of CoNx-graphene for hydrogen evolution. International Journal of Hydrogen Energy, 2018, 43, 20573-20579.	3.8	29
76	Density functional theory study on the interaction of CO with the Fe3O4(001) surface. Applied Surface Science, 2014, 317, 752-759.	3.1	28
77	Effect of Cu doping on the catalytic activity of Fe3O4 in water-gas shift reactions. International Journal of Hydrogen Energy, 2015, 40, 2193-2198.	3.8	28
78	The electronic and reduction properties of Ce0.75Zr0.25O2(110). Chemical Physics Letters, 2008, 450, 286-291.	1.2	27
79	First-Principles Study on the Effects of Zr Dopant on the CO Adsorption on Ceria. Journal of Physical Chemistry C, 2008, 112, 15341-15347.	1.5	27
80	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
81	The mechanism of sulfur poisoning on the nickel/yttrium-stabilized zirconia anode of solid oxide fuel cells: The role of the oxygen vacancy. Journal of Power Sources, 2013, 237, 128-131.	4.0	26
82	Several different charge transfer and Ce³⁺localization scenarios for Rhâ€“CeO₂(111). Journal of Materials Chemistry A, 2014, 2, 2333-2345.	5.2	26
83	Identification of Highâ€Performance Singleâ€Atom MXenes Catalysts for Lowâ€Temperature CO Oxidation. Advanced Theory and Simulations, 2019, 2, 1900006.	1.3	26
84	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. Applied Surface Science, 2019, 479, 590-594.	3.1	26
85	Cooperative Catalysis toward Oxygen Reduction Reaction under Dual Coordination Environments on Intrinsic AMnO₃â€Type Perovskites via Regulating Stacking Configurations of Coordination Units. Advanced Materials, 2020, 32, e2006145.	11.1	26
86	CO₂ Reduction on Metal- and Nitrogen-Codoped Graphene: Balancing Activity and Selectivity via Coordination Engineering. ACS Sustainable Chemistry and Engineering, 2020, 8, 6134-6141.	3.2	26
87	Palladium nanoparticles with high energy facets as a key factor in dissociating O2 in the solvent-free selective oxidation of alcohols. Chemical Communications, 2013, 49, 6626.	2.2	25
88	Tunable Electric Properties of Bilayer Î±-GeTe with Different Interlayer Distances and External Electric Fields. Nanoscale Research Letters, 2018, 13, 400.	3.1	25
89	Adsorption and dissociation of ammonia on small iron clusters. International Journal of Hydrogen Energy, 2015, 40, 346-352.	3.8	23
90	Facile synthesis of silver@carbon nanocable-supported platinum nanoparticles as high-performing electrocatalysts for glycerol oxidation in direct glycerol fuel cells. Green Chemistry, 2016, 18, 386-391.	4.6	23

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91	Coexistence of Type-I and Type-II Weyl Points in the Weyl-Semimetal OsC₂. Journal of Physical Chemistry C, 2018, 122, 3533-3538.	1.5	23
92	Band structure and Fermi surface of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sr</mml:mtext> Physical Review B, 2009, 80, .	1.1	22
93	A theoretical understanding on the CO-tolerance mechanism of the WC(0001) supported Pt monolayer: Some improvement strategies. Applied Surface Science, 2016, 389, 455-461.	3.1	22
94	Dopant segregation and CO adsorption on doped Fe3O4 (1â€¯1â€¯1) surfaces: A first-principle study. Journal of Catalysis, 2018, 364, 291-296.	3.1	22
95	First-principles local density approximation (generalized gradient approximation) +U study of catalytic CenOm clusters: U value differs from bulk. Journal of Chemical Physics, 2008, 128, 164718.	1.2	21
96	Effects of Sm doping content on the ionic conduction of CeO2 in SOFCs from first principles. Applied Physics Letters, 2017, 111, .	1.5	20
97	Strong metalâ€“support interactions impart activity in the oxygen reduction reaction: Au monolayer on Mo₂C (MXene). Journal of Physics Condensed Matter, 2018, 30, 475201.	0.7	20
98	WS₂/BSe van der Waals type-II heterostructure as a promising water splitting photocatalyst. Materials Research Express, 2019, 6, 035513.	0.8	20
99	Sulfidation of Ceria Surfaces from Sulfur and Sulfur Diffusion. Journal of Physical Chemistry C, 2012, 116, 8417-8425.	1.5	19
100	Theoretical Study of the Catalytic CO Oxidation by Pt Catalyst Supported on Ge-Doped Graphene. Journal of Nanoscience and Nanotechnology, 2014, 14, 7117-7124.	0.9	19
101	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
102	Au³⁺ Species Boost the Catalytic Performance of Au/ZnO for the Semi-hydrogenation of Acetylene. ACS Applied Materials & Interfaces, 2021, 13, 40429-40440.	4.0	19
103	Oxygen vacancy induced carbon deposition at the triple phase boundary of the nickel/yttrium-stabilized zirconia (YSZ) interface. Journal of Power Sources, 2014, 261, 136-140.	4.0	18
104	Density functional study on the mechanism for the highly active palladium monolayer supported on titanium carbide for the oxygen reduction reaction. Journal of Chemical Physics, 2016, 144, 204703.	1.2	18
105	The stability of TiC surfaces in the environment with various carbon chemical potential and surface defects. Applied Surface Science, 2016, 386, 202-209.	3.1	18
106	Intrinsic defect-mediated magnetism in Feâ€“N codoped TiO 2. Journal of Alloys and Compounds, 2016, 657, 372-378.	2.8	18
107	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
108	A First-Principles Study of O₂ Dissociation on Platinum Modified Titanium Carbide: A Possible Efficient Catalyst for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2017, 121, 21333-21342.	1.5	18

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109	Design of promising single Rh atom catalyst for CO oxidation based on Graphdiyne sheets. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 130, 114676.	1.3	18
110	First-principles study on the Ni@Pt12 Ih coreâ€“shell nanoparticles: A good catalyst for oxygen reduction reaction. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 3142-3148.	0.9	17
111	High Stability and Reactivity of Pt-Based Coreâ€“Shell Nanoparticles for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2012, 116, 13774-13780.	1.5	17
112	The density functional theory studies on the promoting effect of the Cu-modified Fe 3 O 4 catalysts. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 607-612.	0.9	17
113	Hollow PdCu nanocubes supported by N-doped graphene: A surface science and electrochemical study. International Journal of Hydrogen Energy, 2015, 40, 14305-14313.	3.8	17
114	Effects of a TiC substrate on the catalytic activity of Pt for NO reduction. Physical Chemistry Chemical Physics, 2016, 18, 13304-13309.	1.3	17
115	Substrate effects on the in-plane ferroelectric polarization of two-dimensional SnTe. Physical Review B, 2019, 99, .	1.1	17
116	The carbon-tolerance mechanism of Ni-based alloy with coinage metals. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 2189-2194.	0.9	16
117	Can H2S poison the surface of yttria-stabilized zirconia?. International Journal of Hydrogen Energy, 2013, 38, 8974-8979.	3.8	16
118	Depletion NO x Made Easy by Nitrogen Doped Graphene. Catalysis Letters, 2014, 144, 1016-1022.	1.4	16
119	Importance of oxygen spillover for fuel oxidation on Ni/YSZ anodes in solid oxide fuel cells. Physical Chemistry Chemical Physics, 2014, 16, 8536.	1.3	16
120	Regulation of CO oxidation with Pd additives on Nb2CO2 MXene. International Journal of Hydrogen Energy, 2021, 46, 8477-8485.	3.8	16
121	Interactions of small platinum clusters with the TiC(001) surface. Journal of Applied Physics, 2015, 118, .	1.1	15
122	Novel Ag@C nanocables supported Pd anodes and its implication in energy conversion using direct liquid fuel cells. Applied Energy, 2016, 175, 429-434.	5.1	15
123	A Au monolayer on WC(0001) with unexpected high activity towards CO oxidation. Nanoscale, 2018, 10, 4753-4760.	2.8	15
124	TiC supported single-atom platinum catalyst for CO oxidation: A density functional theory study. Applied Surface Science, 2018, 453, 159-165.	3.1	15
125	The mechanisms for the high resistance to sulfur poisoning of the Ni/yttria-stabilized zirconia system treated with Sn vapor. Physical Chemistry Chemical Physics, 2014, 16, 1033-1040.	1.3	14
126	Understanding on the carbon deposition on the Nickel/Yttriumâ€“Stabilized Zirconia anode caused by the CO containing fuels. Journal of Power Sources, 2015, 279, 759-765.	4.0	14

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127	Resistance to sulfur poisoning of the gold doped nickel/yttria-stabilized zirconia with interface oxygen vacancy. Journal of Power Sources, 2014, 271, 516-521.	4.0	13
128	First principles study on the adsorption of Au dimer on metal-oxide surfaces: The implications for Au growing. Applied Surface Science, 2017, 426, 554-561.	3.1	13
129	First-principles study of adsorption-induced magnetic properties of InSe monolayers. Applied Surface Science, 2018, 436, 419-423.	3.1	13
130	First principles study of the gas sensing 2D GeTe: atomic, electronic and transport properties. Journal Physics D: Applied Physics, 2018, 51, 345304.	1.3	13
131	CO oxidation on MXene (Mo2CS2) supported single-atom catalyst: A termolecular Eley-Rideal mechanism. Chinese Chemical Letters, 2023, 34, 107412.	4.8	13
132	Growth mechanism and controllable synthesis of graphene on Cuâ€“Ni alloy surface in the initial growth stages. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 1361-1365.	0.9	12
133	Effect of Au clustering on ferromagnetism in Au doped TiO2 films: theory and experiments investigation. Journal of Physics and Chemistry of Solids, 2017, 100, 71-77.	1.9	12
134	Activation mechanisms of silver toward CO oxidation by tungsten carbide substrate: A density functional theory study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2436-2442.	0.9	12
135	Au monolayer on WC(0001) with enhanced activity towards NO oxidation: A theoretical study. Applied Surface Science, 2019, 481, 369-373.	3.1	12
136	Sulfur-Doped g-C₃N₄-Supported Ni Species with a Wide Temperature Window for Acetylene Semihydrogenation. ACS Sustainable Chemistry and Engineering, 2022, 10, 4849-4861.	3.2	12
137	O2 activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. Applied Surface Science, 2014, 300, 91-97.	3.1	11
138	Sulfidation and Sulfur Recovery from SO₂ over Ceria. Journal of Physical Chemistry C, 2014, 118, 17499-17504.	1.5	11
139	The sulfur poisoning of the nickel/oxygen-enriched yttria-stabilized zirconia. Journal of Power Sources, 2015, 293, 635-641.	4.0	11
140	Resistance to sulfur poisoning of Ni-based alloy with coinage (IB) metals. Applied Surface Science, 2015, 357, 1785-1791.	3.1	11
141	A first principles study of O2 dissociation on Pt modified ZrC(100) surface. Chemical Physics Letters, 2016, 649, 141-147.	1.2	11
142	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
143	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. Applied Surface Science, 2017, 394, 47-57.	3.1	11
144	Investigations on the origin of ferromagnetism of Cu doped anatase TiO 2 nanotubes. Materials Research Bulletin, 2017, 86, 287-294.	2.7	11

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145	TiC and TiN supported platinum monolayer as high-performance catalysts for CO oxidation: A DFT study. Journal of Chemical Physics, 2018, 149, 054705.	1.2	11
146	Design of Highly Stable and Efficient Bifunctional MX ene-Based Electrocatalysts for Oxygen Reduction and Evolution Reactions. Physical Review Applied, 2021, 15, .	1.5	11
147	First-principles study on the orbital ordering of KCrF3. Physical Review B, 2011, 84, .	1.1	10
148	First-principles study on the mechanism of coking inhibition by the Ni(111) surface doped with IB-group metals at the anode of solid oxide fuel cells. Journal of Power Sources, 2013, 242, 762-767.	4.0	10
149	Design of Efficient Catalysts for CO Oxidation on Titanium Carbide-Supported Platinum via Computational Study. Journal of Physical Chemistry C, 2018, 122, 25974-25982.	1.5	10
150	High activity of Au monolayer doped by Pt atom on WC (0001) surface towards H2 dissociation and high tolerance of sulfur poisoning. Journal of Alloys and Compounds, 2019, 775, 330-334.	2.8	10
151	Improved oxygen reduction activity on the Ih Cu@Pt coreâ€“shell nanoparticles. Chemical Physics Letters, 2011, 513, 118-123.	1.2	9
152	Unusual Stability and Activity of DI-Pd19 Clusters for O₂ Dissociation. Journal of Physical Chemistry C, 2012, 116, 19586-19589.	1.5	9
153	Tuning the catalytic activity of Agâ€“Pd alloy cluster for hydrogen dissociation by controlling the Pd ratio. Computational and Theoretical Chemistry, 2015, 1071, 39-45.	1.1	9
154	The first principles study of the sulfur oxidation on Ni surface with H2O. Journal of Alloys and Compounds, 2018, 741, 1183-1187.	2.8	9
155	Ag monolayer doped by Pt atom on WC (0001) surface: A good catalyst for H2 dissociation with high sulfur tolerance. International Journal of Hydrogen Energy, 2019, 44, 3115-3120.	3.8	9
156	First-principles study on the Cu-Au alloy monolayer supported on WC for hydrogen evolution. Applied Surface Science, 2021, 565, 150568.	3.1	9
157	The effect of Zr-doping on the interaction of water molecules with the ceria (111) surface. Surface Science, 2011, 605, 351-360.	0.8	8
158	The highly active Ce4O8 nanoparticle for CO oxidation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 3235-3240.	0.9	8
159	First-principles investigation of H₂S adsorption and dissociation on titanium carbide surfaces. Physical Chemistry Chemical Physics, 2017, 19, 27116-27122.	1.3	8
160	Screening the best catalyst with group 9, 10 and 11 metals monolayer loading on NbC(001) from first-principles study. Journal of Power Sources, 2018, 378, 691-698.	4.0	8
161	High Stability and Reactivity of Single-Metal Atom Catalysts Supported on Yttria-Stabilized Zirconia: The Role of the Surface Oxygen Vacancy. Journal of Physical Chemistry C, 2018, 122, 1622-1630.	1.5	8
162	The mechanism of the high resistance to sulfur poisoning of the rhenium doped nickel/yttria-stabilized zirconia. Applied Surface Science, 2018, 447, 561-568.	3.1	8

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163	Understanding the correlation between the electronic structure and catalytic behavior of TiC(001) and TiN(001) surfaces: DFT study. Applied Surface Science, 2019, 494, 57-62.	3.1	8
164	Efficient band structure engineering and visible-light response in ZrS2/GaS heterobilayer by electrical field or external strains. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2969-2973.	0.9	8
165	An electronic perturbation in TiC supported platinum monolayer catalyst for enhancing waterâ€“gas shift performance: DFT study. Journal of Physics Condensed Matter, 2019, 31, 305201.	0.7	8
166	The electronic structure and magnetism of KxFe2Se2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 1072-1077.	0.9	7
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