

Zongxian Yang

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209
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212
ext. papers

7,032
ext. citations

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avg, IF

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L-index

#	Paper	IF	Citations
209	Atomic and electronic structure of unreduced and reduced CeO ₂ surfaces: a first-principles study. <i>Journal of Chemical Physics</i> , 2004 , 120, 7741-9	3.9	304
208	A theoretical simulation on the catalytic oxidation of CO on Pt/graphene. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 16566-72	3.6	266
207	The adsorption of CO and NO on the MoS ₂ monolayer doped with Au, Pt, Pd, or Ni: A first-principles study. <i>Applied Surface Science</i> , 2016 , 383, 98-105	6.7	223
206	Bifunctional Co _{Nx} embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. <i>Carbon</i> , 2018 , 130, 112-119	10.4	149
205	Novel catalytic activity for oxygen reduction reaction on MnN ₄ embedded graphene: A dispersion-corrected density functional theory study. <i>Carbon</i> , 2015 , 84, 500-508	10.4	147
204	The mechanisms of oxygen reduction reaction on phosphorus doped graphene: A first-principles study. <i>Journal of Power Sources</i> , 2015 , 276, 222-229	8.9	133
203	3d transition metal embedded C ₂ N monolayers as promising single-atom catalysts: A first-principles study. <i>Carbon</i> , 2016 , 105, 463-473	10.4	132
202	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. <i>Carbon</i> , 2017 , 118, 35-42	10.4	126
201	C ₃ N monolayers as promising candidates for NO ₂ sensors. <i>Sensors and Actuators B: Chemical</i> , 2018 , 266, 664-673	8.5	126
200	Modulating electronic, magnetic and chemical properties of MoS ₂ monolayer sheets by substitutional doping with transition metals. <i>Applied Surface Science</i> , 2016 , 364, 181-189	6.7	120
199	Effects of Zr doping on stoichiometric and reduced ceria: a first-principles study. <i>Journal of Chemical Physics</i> , 2006 , 124, 224704	3.9	113
198	Trapping of metal atoms in the defects on graphene. <i>Journal of Chemical Physics</i> , 2011 , 135, 224704	3.9	104
197	Theoretical study on the Si-doped graphene as an efficient metal-free catalyst for CO oxidation. <i>Applied Surface Science</i> , 2014 , 308, 402-407	6.7	100
196	Physisorbed, Chemisorbed, and Oxidized CO on Highly Active Cu ₂ CeO ₂ (111). <i>Journal of Physical Chemistry C</i> , 2010 , 114, 4486-4494	3.8	99
195	Formaldehyde molecule adsorption on the doped monolayer MoS ₂ : A first-principles study. <i>Applied Surface Science</i> , 2016 , 371, 180-188	6.7	99
194	The Effect of Environment on the Reaction of Water on the Ceria(111) Surface: A DFT+U Study. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 14891-14899	3.8	96
193	Strong and weak adsorption of CO on CeO ₂ surfaces from first principles calculations. <i>Chemical Physics Letters</i> , 2004 , 396, 384-392	2.5	95

192	Oxygen vacancy formation energy in Pd-doped ceria: a DFT+U study. <i>Journal of Chemical Physics</i> , 2007 , 127, 074704	3.9	90
191	Repairing sulfur vacancies in the MoS ₂ monolayer by using CO, NO and NO ₂ molecules. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 7093-7101	7.1	88
190	A promising single atom catalyst for CO oxidation: Ag on boron vacancies of h-BN sheets. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16795-16805	3.6	84
189	CO oxidation catalyzed by the single Co atom embedded hexagonal boron nitride nanosheet: a DFT-D study. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 21865-70	3.6	81
188	First principles study on the interfacial properties of NM/graphdiyne (NM = Pd, Pt, Rh and Ir): The implications for NM growing. <i>Applied Surface Science</i> , 2016 , 360, 1-7	6.7	78
187	Tuning the catalytic property of non-noble metallic impurities in graphene. <i>Carbon</i> , 2014 , 71, 139-149	10.4	78
186	Single Pt atom stabilized on nitrogen doped graphene: CO oxidation readily occurs via the tri-molecular Eley-Rideal mechanism. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 20006-13	3.6	76
185	CO oxidation on Mn-N ₄ porphyrin-like carbon nanotube: A DFT-D study. <i>Applied Surface Science</i> , 2017 , 426, 1232-1240	6.7	75
184	Formation and catalytic activity of Pt supported on oxidized graphene for the CO oxidation reaction. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 7887-95	3.6	73
183	First-principles study of the Pt/CeO ₂ (111) interface. <i>Physical Review B</i> , 2007 , 76,	3.3	73
182	Formation, Stabilities, and Electronic and Catalytic Performance of Platinum Catalyst Supported on Non-Metal-Doped Graphene. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5258-5268	3.8	71
181	Oxygen vacancy formation energy at the Pd/CeO ₂ (111) interface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2007 , 369, 132-139	2.3	63
180	First-Principles Study on the Single Ir Atom Embedded Graphdiyne: An Efficient Catalyst for CO Oxidation. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 23481-23492	3.8	63
179	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. <i>Surface Science</i> , 2008 , 602, 1199-1206	1.8	61
178	Single non-noble-metal cobalt atom stabilized by pyridinic vacancy graphene: An efficient catalyst for CO oxidation. <i>Journal of Molecular Catalysis A</i> , 2016 , 417, 28-35		60
177	Facile synthesis of hollow palladium/copper alloyed nanocubes for formic acid oxidation. <i>Chemical Communications</i> , 2011 , 47, 8581-3	5.8	59
176	Pd ₁ /BN as a promising single atom catalyst of CO oxidation: a dispersion-corrected density functional theory study. <i>RSC Advances</i> , 2015 , 5, 84381-84388	3.7	56
175	Single Pd atomic catalyst on MoCO monolayer (MXene): unusual activity for CO oxidation by trimolecular Eley-Rideal mechanism. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 3504-3513	3.6	56

174	A density function theory study on the NO reduction on nitrogen doped graphene. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 20561-9	3.6	49
173	Boron-Doped C3N Monolayer as a Promising Metal-Free Oxygen Reduction Reaction Catalyst: A Theoretical Insight. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 20312-20322	3.8	48
172	Origin of the High Activity of the Ceria-Supported Copper Catalyst for H ₂ O Dissociation. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 6730-6740	3.8	48
171	First-principles study of the adsorption of sulfur on Pt(111): S core-level shifts and the nature of the Pt-S bond. <i>Physical Review B</i> , 2002 , 65,	3.3	47
170	The sensing mechanism of Pt-doped SnO ₂ surface toward CO: A first-principle study. <i>Sensors and Actuators B: Chemical</i> , 2014 , 202, 83-92	8.5	45
169	Cu-doped ceria: Oxygen vacancy formation made easy. <i>Chemical Physics Letters</i> , 2011 , 510, 60-66	2.5	45
168	3D well-ordered porous phosphorus doped carbon as an anode for sodium storage: structure design, experimental and computational insights. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 11400-11407 ¹³		42
167	Interaction between HO, N, CO, NO, NO and NO molecules and a defective WSe monolayer. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 26022-26033	3.6	42
166	Direct CO oxidation by lattice oxygen on the SnO ₂ (110) surface: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 12488-94	3.6	40
165	Noble metals induced magnetic properties of graphene. <i>Journal of Magnetism and Magnetic Materials</i> , 2011 , 323, 2441-2447	2.8	39
164	The mechanism of oxygen reduction reaction on CoN ₄ embedded graphene: A combined kinetic and atomistic thermodynamic study. <i>International Journal of Hydrogen Energy</i> , 2016 , 41, 21212-21220	6.7	39
163	Cu-Cluster-Doped Monolayer MoCO (MXene) as an Electron Reservoir for Catalyzing a CO Oxidation Reaction. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 32903-32912	9.5	38
162	Sulfur doped graphene as a promising metal-free electrocatalyst for oxygen reduction reaction: a DFT-D study. <i>RSC Advances</i> , 2017 , 7, 20398-20405	3.7	37
161	Oxygen vacancy pairs on CeO ₂ (110): A DFT + U study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009 , 373, 2786-2792	2.3	37
160	Structural and electronic properties of NM-doped ceria (NM = Pt, Rh): a first-principles study. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 035210	1.8	36
159	Repairing single and double atomic vacancies in a CN monolayer with CO or NO molecules: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 13517-13527	3.6	34
158	Detection of gas molecules on single Mn adatom adsorbed graphyne: a DFT-D study. <i>Journal Physics D: Applied Physics</i> , 2018 , 51, 065109	3	34
157	Preventing the CO poisoning on Pt nanocatalyst using appropriate substrate: a first-principles study. <i>Journal of Nanoparticle Research</i> , 2012 , 14, 1	2.3	32

156	The adsorption, diffusion and dissociation of O ₂ on Pt-skin Pt ₃ Ni(111): A density functional theory study. <i>Chemical Physics Letters</i> , 2010 , 499, 83-88	2.5	32
155	A comparison study of oxygen reduction on the supported Pt, Pd, Au monolayer on WC(0001). <i>Journal of Power Sources</i> , 2016 , 321, 163-173	8.9	31
154	Direct CO Oxidation by Lattice Oxygen on Zr-Doped Ceria Surfaces. <i>Catalysis Letters</i> , 2011 , 141, 78-82	2.8	31
153	Additive-free fabrication of spherical hollow palladium/copper alloyed nanostructures for fuel cell application. <i>ACS Applied Materials & Interfaces</i> , 2012 , 4, 4461-4	9.5	30
152	SO _x on ceria from adsorbed SO ₂ . <i>Journal of Chemical Physics</i> , 2011 , 134, 184703	3.9	30
151	Interfacial properties of NM/CeO ₂ (111) (NM = noble metal atoms or clusters of Pd, Pt and Rh): a first principles study. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 475003	1.8	29
150	Density functional theory studies on the adsorption, diffusion and dissociation of O ₂ on Pt(111). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010 , 374, 4713-4717	2.3	29
149	The synergistic effects of the Cu-CeO ₂ (111) catalysts on the adsorption and dissociation of water molecules. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 9363-73	3.6	28
148	Density Functional Theory Study of Sn Adsorption on the CeO ₂ Surface. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 16461-16466	3.8	28
147	Theoretical Inspection of M1/PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). <i>ACS Catalysis</i> , 2021 , 11, 8929-8941	13.1	28
146	First-Principles Study on the Effects of Zr Dopant on the CO Adsorption on Ceria. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 15341-15347	3.8	26
145	Several different charge transfer and Ce ³⁺ localization scenarios for Rh/CeO ₂ (111). <i>Journal of Materials Chemistry A</i> , 2014 , 2, 2333-2345	13	24
144	Density functional theory study on the interaction of CO with the Fe ₃ O ₄ (001) surface. <i>Applied Surface Science</i> , 2014 , 317, 752-759	6.7	24
143	The mechanism of sulfur poisoning on the nickel/yttrium-stabilized zirconia anode of solid oxide fuel cells: The role of the oxygen vacancy. <i>Journal of Power Sources</i> , 2013 , 237, 128-131	8.9	24
142	Effect of Cu doping on the catalytic activity of Fe ₃ O ₄ in water-gas shift reactions. <i>International Journal of Hydrogen Energy</i> , 2015 , 40, 2193-2198	6.7	24
141	The mechanism of oxygen activation on single Pt-atom doped SnO ₂ (110) surface. <i>Journal of Materials Science</i> , 2016 , 51, 10400-10407	4.3	24
140	Novel two-dimensional ferroelectric PbTe under tension: A first-principles prediction. <i>Journal of Applied Physics</i> , 2017 , 122, 064101	2.5	22
139	Electronic structure and optical properties for blue phosphorene/graphene-like GaN van der Waals heterostructures. <i>Current Applied Physics</i> , 2017 , 17, 1714-1720	2.6	21

138	Palladium nanoparticles with high energy facets as a key factor in dissociating O ₂ in the solvent-free selective oxidation of alcohols. <i>Chemical Communications</i> , 2013 , 49, 6626-8	5.8	21
137	Band structure and Fermi surface of (Sr ₂ VO ₃) ₂ Fe ₂ As ₂ and (Sr ₂ ScO ₃) ₂ Fe ₂ As ₂ . <i>Physical Review B</i> , 2009 , 80,	3.3	21
136	The electronic and reduction properties of Ce _{0.75} Zr _{0.25} O ₂ (110). <i>Chemical Physics Letters</i> , 2008 , 450, 286-291	2.5	21
135	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. <i>Applied Surface Science</i> , 2019 , 479, 590-594	6.7	21
134	Engineering the activity of Co _{Nx} -graphene for hydrogen evolution. <i>International Journal of Hydrogen Energy</i> , 2018 , 43, 20573-20579	6.7	21
133	CO ₂ thermoreduction to methanol on the MoS ₂ supported single Co atom catalyst: A DFT study. <i>Applied Surface Science</i> , 2020 , 528, 147047	6.7	20
132	The role of the intrinsic Se and In vacancies in the interaction of O ₂ and H ₂ O molecules with the InSe monolayer. <i>Applied Surface Science</i> , 2018 , 434, 215-227	6.7	20
131	First-principles local density approximation (generalized gradient approximation) +U study of catalytic Ce _n O _m clusters: U value differs from bulk. <i>Journal of Chemical Physics</i> , 2008 , 128, 164718	3.9	20
130	Theoretical study of the catalytic CO oxidation by Pt catalyst supported on Ge-doped grapheme. <i>Journal of Nanoscience and Nanotechnology</i> , 2014 , 14, 7117-24	1.3	19
129	Tunable magnetic and electronic properties of the Cr-based MXene (Cr ₂ C) with functional groups and doping. <i>Journal of Magnetism and Magnetic Materials</i> , 2020 , 514, 167141	2.8	18
128	Tuning metal cluster catalytic activity with morphology and composition: a DFT study of O ₂ dissociation at the global minimum of Pt _m Pd _n (m + n = 5) clusters. <i>RSC Advances</i> , 2016 , 6, 104388-104397	3.7	18
127	Dopant segregation and CO adsorption on doped Fe ₃ O ₄ (1 1 1) surfaces: A first-principle study. <i>Journal of Catalysis</i> , 2018 , 364, 291-296	7.3	18
126	Sulfidation of Ceria Surfaces from Sulfur and Sulfur Diffusion. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 8417-8425	3.8	18
125	Strong metal-support interactions impart activity in the oxygen reduction reaction: Au monolayer on MoC (MXene). <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 475201	1.8	18
124	High Stability and Reactivity of Pt-Based CoreShell Nanoparticles for Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 13774-13780	3.8	17
123	Recent progress of MXenes as the support of catalysts for the CO oxidation and oxygen reduction reaction. <i>Chinese Chemical Letters</i> , 2020 , 31, 931-936	8.1	17
122	Density functional study on the mechanism for the highly active palladium monolayer supported on titanium carbide for the oxygen reduction reaction. <i>Journal of Chemical Physics</i> , 2016 , 144, 204703	3.9	17
121	Effects of rare-earth doping on the ionic conduction of CeO ₂ in solid oxide fuel cells. <i>Ceramics International</i> , 2018 , 44, 3707-3711	5.1	17

120	Tunable Electric Properties of Bilayer HgTe with Different Interlayer Distances and External Electric Fields. <i>Nanoscale Research Letters</i> , 2018 , 13, 400	5	17
119	Facile synthesis of silver@carbon nanocable-supported platinum nanoparticles as high-performing electrocatalysts for glycerol oxidation in direct glycerol fuel cells. <i>Green Chemistry</i> , 2016 , 18, 386-391	10	16
118	Depletion NO _x Made Easy by Nitrogen Doped Graphene. <i>Catalysis Letters</i> , 2014 , 144, 1016-1022	2.8	16
117	A First-Principles Study of O ₂ Dissociation on Platinum Modified Titanium Carbide: A Possible Efficient Catalyst for the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 21333-21342	3.8	16
116	Effects of Sm doping content on the ionic conduction of CeO ₂ in SOFCs from first principles. <i>Applied Physics Letters</i> , 2017 , 111, 023903	3.4	16
115	A theoretical understanding on the CO-tolerance mechanism of the WC(0001) supported Pt monolayer: Some improvement strategies. <i>Applied Surface Science</i> , 2016 , 389, 455-461	6.7	16
114	Identification of High-Performance Single-Atom MXenes Catalysts for Low-Temperature CO Oxidation. <i>Advanced Theory and Simulations</i> , 2019 , 2, 1900006	3.5	15
113	Adsorption and dissociation of ammonia on small iron clusters. <i>International Journal of Hydrogen Energy</i> , 2015 , 40, 346-352	6.7	15
112	Tailoring the Electronic Structure of Transition Metals by the VC MXene Support: Excellent Oxygen Reduction Performance Triggered by Metal-Support Interactions. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 28206-28216	9.5	15
111	CO ₂ Reduction on Metal- and Nitrogen-Codoped Graphene: Balancing Activity and Selectivity via Coordination Engineering. <i>ACS Sustainable Chemistry and Engineering</i> , 2020 , 8, 6134-6141	8.3	15
110	Identification of Efficient Single-Atom Catalysts Based on V ₂ CO ₂ MXene by ab Initio Simulations. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 4090-4100	3.8	15
109	Coexistence of Type-I and Type-II Weyl Points in the Weyl-Semimetal OsC ₂ . <i>Journal of Physical Chemistry C</i> , 2018 , 122, 3533-3538	3.8	15
108	Intrinsic defect-mediated magnetism in Fe _N codoped TiO ₂ . <i>Journal of Alloys and Compounds</i> , 2016 , 657, 372-378	5.7	15
107	Oxygen vacancy induced carbon deposition at the triple phase boundary of the nickel/yttrium-stabilized zirconia (YSZ) interface. <i>Journal of Power Sources</i> , 2014 , 261, 136-140	8.9	15
106	The carbon-tolerance mechanism of Ni-based alloy with coinage metals. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013 , 377, 2189-2194	2.3	15
105	The density functional theory studies on the promoting effect of the Cu-modified Fe ₃ O ₄ catalysts. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015 , 379, 607-612	2.3	15
104	Can H ₂ S poison the surface of yttria-stabilized zirconia?. <i>International Journal of Hydrogen Energy</i> , 2013 , 38, 8974-8979	6.7	15
103	First-principles study on the Ni@Pt ₁₂ Ih core-shell nanoparticles: A good catalyst for oxygen reduction reaction. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011 , 375, 3142-3148	2.3	15

102	Hollow PdCu nanocubes supported by N-doped graphene: A surface science and electrochemical study. <i>International Journal of Hydrogen Energy</i> , 2015 , 40, 14305-14313	6.7	14
101	Interactions of small platinum clusters with the TiC(001) surface. <i>Journal of Applied Physics</i> , 2015 , 118, 185301	2.5	14
100	Understanding on the carbon deposition on the Nickel/Yttrium-stabilized Zirconia anode caused by the CO containing fuels. <i>Journal of Power Sources</i> , 2015 , 279, 759-765	8.9	14
99	Effects of a TiC substrate on the catalytic activity of Pt for NO reduction. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 13304-9	3.6	14
98	TiC supported single-atom platinum catalyst for CO oxidation: A density functional theory study. <i>Applied Surface Science</i> , 2018 , 453, 159-165	6.7	14
97	Mechanisms of direct hydrogen peroxide synthesis on silicon and phosphorus dual-doped graphene: a DFT-D study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 9007-9015	3.6	13
96	Novel Ag@C nanocables supported Pd anodes and its implication in energy conversion using direct liquid fuel cells. <i>Applied Energy</i> , 2016 , 175, 429-434	10.7	13
95	The mechanisms for the high resistance to sulfur poisoning of the Ni/yttria-stabilized zirconia system treated with Sn vapor. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 1033-40	3.6	13
94	Tuning the ORR activity of Pt-based TiCO MXenes by varying the atomic cluster size and doping with metals. <i>Nanoscale</i> , 2020 , 12, 12497-12507	7.7	12
93	A Au monolayer on WC(0001) with unexpected high activity towards CO oxidation. <i>Nanoscale</i> , 2018 , 10, 4753-4760	7.7	12
92	The stability of TiC surfaces in the environment with various carbon chemical potential and surface defects. <i>Applied Surface Science</i> , 2016 , 386, 202-209	6.7	12
91	Resistance to sulfur poisoning of the gold doped nickel/yttria-stabilized zirconia with interface oxygen vacancy. <i>Journal of Power Sources</i> , 2014 , 271, 516-521	8.9	12
90	Importance of oxygen spillover for fuel oxidation on Ni/YSZ anodes in solid oxide fuel cells. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 8536-40	3.6	12
89	WS ₂ /BSe van der Waals type-II heterostructure as a promising water splitting photocatalyst. <i>Materials Research Express</i> , 2019 , 6, 035513	1.7	12
88	First-principles study of adsorption-induced magnetic properties of InSe monolayers. <i>Applied Surface Science</i> , 2018 , 436, 419-423	6.7	12
87	Growth mechanism and controllable synthesis of graphene on Cu ₃ Ni alloy surface in the initial growth stages. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015 , 379, 1361-1365	2.3	11
86	Sulfidation and Sulfur Recovery from SO ₂ over Ceria. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 17499-17504	3.5	11
85	First principles study on the adsorption of Au dimer on metal-oxide surfaces: The implications for Au growing. <i>Applied Surface Science</i> , 2017 , 426, 554-561	6.7	11

84	Design of promising single Rh atom catalyst for CO oxidation based on Graphdiyne sheets. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 130, 114676	3	11
83	Substrate effects on the in-plane ferroelectric polarization of two-dimensional SnTe. <i>Physical Review B</i> , 2019 , 99,	3.3	10
82	Au monolayer on WC(0001) with enhanced activity towards NO oxidation: A theoretical study. <i>Applied Surface Science</i> , 2019 , 481, 369-373	6.7	10
81	A first principles study of O ₂ dissociation on Pt modified ZrC(100) surface. <i>Chemical Physics Letters</i> , 2016 , 649, 141-147	2.5	10
80	Cooperative Catalysis toward Oxygen Reduction Reaction under Dual Coordination Environments on Intrinsic AMnO _x -Type Perovskites via Regulating Stacking Configurations of Coordination Units. <i>Advanced Materials</i> , 2020 , 32, e2006145	24	10
79	First principles study of the gas sensing 2D GeTe: atomic, electronic and transport properties. <i>Journal Physics D: Applied Physics</i> , 2018 , 51, 345304	3	9
78	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. <i>Applied Surface Science</i> , 2017 , 394, 47-57	6.7	9
77	Investigations on the origin of ferromagnetism of Cu doped anatase TiO ₂ nanotubes. <i>Materials Research Bulletin</i> , 2017 , 86, 287-294	5.1	9
76	The sulfur poisoning of the nickel/oxygen-enriched yttria-stabilized zirconia. <i>Journal of Power Sources</i> , 2015 , 293, 635-641	8.9	9
75	Resistance to sulfur poisoning of Ni-based alloy with coinage (IB) metals. <i>Applied Surface Science</i> , 2015 , 357, 1785-1791	6.7	9
74	Unusual Stability and Activity of DI-Pd ₁₉ Clusters for O ₂ Dissociation. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 19586-19589	3.8	9
73	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. <i>Journal of Power Sources</i> , 2013 , 242, 762-767	8.9	9
72	Tuning the catalytic activity of AgPd alloy cluster for hydrogen dissociation by controlling the Pd ratio. <i>Computational and Theoretical Chemistry</i> , 2015 , 1071, 39-45	2	8
71	Effect of Au clustering on ferromagnetism in Au doped TiO ₂ films: theory and experiments investigation. <i>Journal of Physics and Chemistry of Solids</i> , 2017 , 100, 71-77	3.9	8
70	O ₂ activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. <i>Applied Surface Science</i> , 2014 , 300, 91-97	6.7	8
69	Improved oxygen reduction activity on the Ih Cu@Pt core-shell nanoparticles. <i>Chemical Physics Letters</i> , 2011 , 513, 118-123	2.5	8
68	First-principles study on the orbital ordering of KCrF ₃ . <i>Physical Review B</i> , 2011 , 84,	3.3	8
67	Design of Efficient Catalysts for CO Oxidation on Titanium Carbide-Supported Platinum via Computational Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 25974-25982	3.8	8

66	The first principles study of the sulfur oxidation on Ni surface with H ₂ O. <i>Journal of Alloys and Compounds</i> , 2018 , 741, 1183-1187	5.7	7
65	TiC and TiN supported platinum monolayer as high-performance catalysts for CO oxidation: A DFT study. <i>Journal of Chemical Physics</i> , 2018 , 149, 054705	3.9	7
64	Tuning the Physical and Chemical Properties of 2D InSe with Interstitial Boron Doping: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 28312-28316	3.8	7
63	The highly active Ce ₄ O ₈ nanoparticle for CO oxidation. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 3235-3240	2.3	7
62	The effect of Zr-doping on the interaction of water molecules with the ceria (111) surface. <i>Surface Science</i> , 2011 , 605, 351-360	1.8	7
61	Ag monolayer doped by Pt atom on WC (0001) surface: A good catalyst for H ₂ dissociation with high sulfur tolerance. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 3115-3120	6.7	7
60	High activity of Au monolayer doped by Pt atom on WC (0001) surface towards H ₂ dissociation and high tolerance of sulfur poisoning. <i>Journal of Alloys and Compounds</i> , 2019 , 775, 330-334	5.7	7
59	Activation mechanisms of silver toward CO oxidation by tungsten carbide substrate: A density functional theory study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019 , 383, 2436-2442 ⁶	2.3	6
58	The adsorption and dissociation of O ₂ on Pd and Pt modified TaC (1 0 0) surface: A first principles study. <i>Applied Surface Science</i> , 2018 , 439, 845-851	6.7	6
57	High Stability and Reactivity of Single-Metal Atom Catalysts Supported on Yttria-Stabilized Zirconia: The Role of the Surface Oxygen Vacancy. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 1622-1630	3.8	6
56	The mechanism of the high resistance to sulfur poisoning of the rhenium doped nickel/yttria-stabilized zirconia. <i>Applied Surface Science</i> , 2018 , 447, 561-568	6.7	6
55	Low-temperature preferential oxidation of CO over Ag monolayer decorated MoC (MXene) for purifying H ₂ . <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 215201	1.8	6
54	Cr ₂ NX ₂ MXene (X = O, F, OH): A 2D ferromagnetic half-metal. <i>Applied Physics Letters</i> , 2021 , 119, 062404 ^{3,4}	3.4	6
53	Efficient noble metal nanocatalysts supported on HfC(001) for O ₂ dissociation. <i>AIP Advances</i> , 2017 , 7, 035015	1.5	5
52	Screening the best catalyst with group 9, 10 and 11 metals monolayer loading on NbC(001) from first-principles study. <i>Journal of Power Sources</i> , 2018 , 378, 691-698	8.9	5
51	The possible magnetoelectric coupling induced by adsorption in SnTe films. <i>Applied Surface Science</i> , 2018 , 428, 89-93	6.7	5
50	The search for the good Pd-based catalyst for oxygen reduction reaction: core-shell M ₄ @Pd ₂₀ nanowires. <i>Journal of Nanoparticle Research</i> , 2014 , 16, 1	2.3	5
49	Highly efficient Pd-based core-shell nanowire catalysts for O ₂ dissociation. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 20532-6	3.6	5

48	The sulfur tolerance mechanism of the Cu/CeO ₂ system. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 1957-1966	6.7	5
47	The electronic structure and magnetism of KxFe ₂ Se ₂ . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 1072-1077	2.3	5
46	The formation and properties of Pt ₄ clusters on the defective graphene support. <i>Journal of Nanoscience and Nanotechnology</i> , 2013 , 13, 1612-5	1.3	5
45	An electronic perturbation in TiC supported platinum monolayer catalyst for enhancing water-gas shift performance: DFT study. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 305201	1.8	5
44	A possible highly active supported Ni dimer catalyst for O ₂ dissociation: A first-principles study. <i>Applied Surface Science</i> , 2017 , 402, 168-174	6.7	4
43	Efficient band structure engineering and visible-light response in ZrS ₂ /GaS heterobilayer by electrical field or external strains. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019 , 383, 2969-2973	2.3	4
42	Adsorption and oxidation of sulfur dioxide on the yttria-stabilized zirconia surface: ab initio atomistic thermodynamics study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014 , 378, 659-666	2.3	4
41	The origin of the low efficiency of carbon removal from the Nickel/Yttrium Stabilized Zirconia triple-phase boundary by adsorbed water. <i>Journal of Power Sources</i> , 2015 , 279, 224-230	8.9	4
40	Comparative study of the magnetism of SrTcO ₃ and Ca(Sr)MnO ₃ . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 3313-3316	2.3	4
39	Orbital ordering in Mott-insulators La ₂ O ₃ Fe ₂ Se ₂ and La ₂ O ₃ Co ₂ Se ₂ . <i>Solid State Communications</i> , 2011 , 151, 1231-1235	1.6	4
38	Potential parent compound of superconductor: Sr ₂ CuM ₂ As ₂ O ₂ (M=Mn, Fe). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010 , 374, 4727-4731	2.3	4
37	Enhanced sulfur resistance of Ni(1 1 1) surface alloyed with Ge: A first principles study. <i>Surface Science</i> , 2018 , 677, 115-120	1.8	4
36	First-principles investigation of HS adsorption and dissociation on titanium carbide surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 27116-27122	3.6	3
35	Microstructure and magnetic properties of In _{1-x} CrxN thin films. <i>Materials Science in Semiconductor Processing</i> , 2015 , 31, 147-152	4.3	3
34	First-principles study for the enhanced sulfur tolerance of Ni(100) surface alloyed with Pb. <i>Surface Science</i> , 2018 , 670, 68-71	1.8	3
33	Understanding the correlation between the electronic structure and catalytic behavior of TiC(001) and TiN(001) surfaces: DFT study. <i>Applied Surface Science</i> , 2019 , 494, 57-62	6.7	3
32	Effects of substrate defects on the carbon cluster formation in graphene growth on Ni(111) surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014 , 378, 3055-3059	2.3	3
31	First-Principles Study on the Initial Oxidization of a Nb(100) Surface. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 23371-23376	3.8	3

30	Cooperative activation effect on H ₂ O adsorption in MnO _x catalyzed steam methane reforming. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019 , 383, 1357-1361	2.3	3
29	Effects of Si-doping on magnetic properties of Ga _{1-x} Cr _x N. <i>Journal of Magnetism and Magnetic Materials</i> , 2015 , 374, 564-568	2.8	2
28	Density functional study on the high catalytic performance of single metal atoms on the NbC(001) surface. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 10302-10310	3.6	2
27	The electronic structure of LaCo ₂ B ₂ . <i>Europhysics Letters</i> , 2011 , 95, 17001	1.6	2
26	The Adsorption of Ag and Sb on Ag(111) Surface. <i>Physica Status Solidi (B): Basic Research</i> , 1999 , 212, 281-285		2
25	Efficient metal overlayer catalysts on the NbC monolayer for CO oxidation from first-principles screening. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 175201	1.8	2
24	Design of Highly Stable and Efficient Bifunctional MXene-Based Electrocatalysts for Oxygen Reduction and Evolution Reactions. <i>Physical Review Applied</i> , 2021 , 15,	4.3	2
23	Regulation of CO oxidation with Pd additives on Nb ₂ CO ₂ MXene. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 8477-8485	6.7	2
22	Ultrafast Kinetics in a PAN/MgFeO Flexible Free-Standing Anode Induced by Heterojunction and Oxygen Vacancies.. <i>ACS Applied Materials & Interfaces</i> , 2022 ,	9.5	2
21	High resistance to sulfur poisoning of Ni with copper skin under electric field. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017 , 381, 671-678	2.3	1
20	A theoretical study of the lowest-energy PtPd co-doped silicon clusters: Chirality and fluxional transformation. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017 , 381, 873-878	2.3	1
19	Investigations on the origin of ferromagnetism in Ga _{1-x} Cr _x N and Si-doped Ga _{1-x} Cr _x N films: Experiments and theory. <i>Journal of Alloys and Compounds</i> , 2016 , 658, 800-805	5.7	1
18	Ab initio atomistic thermodynamics study on the sulfur tolerance mechanism of the oxygen-enriched yttria-stabilized zirconia surface. <i>Surface Science</i> , 2014 , 622, 16-23	1.8	1
17	Accelerating oxygen reduction on Pt monolayer via substrate compression. <i>Journal Physics D: Applied Physics</i> , 2017 , 50, 435501	3	1
16	Density functional study on the resistance to sulfur poisoning of Pt (x = 0, 1, 4 and 8) modified TiMoC(0001) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 24879-24885	3.6	1
15	The catalysis mechanism of noble metals at electronic level. <i>Journal of Nanoscience and Nanotechnology</i> , 2010 , 10, 7816-9	1.3	1
14	Mitigation of CO poisoning on functionalized palladium monolayer supported on titanium carbide. <i>Surface and Coatings Technology</i> , 2020 , 402, 125925	4.4	1
13	Manipulation of electronic and magnetic properties of Cr ₂ CX ₂ (X=F,O,OH) monolayer by applying mechanical strains. <i>Journal of Alloys and Compounds</i> , 2021 , 850, 156769	5.7	1

12	Substitution of Fe in hydroxyapatite as an efficient single-atom catalyst for oxygen reduction reaction in biofuel cells: A first-principles study. <i>Applied Surface Science</i> , 2021 , 539, 148233	6.7	1
11	Modulating oxygen electronic orbital occupancy of Cr-based MXenes via transition metal adsorbing for optimal HER activity. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 25457-25467	6.7	1
10	Au Species Boost the Catalytic Performance of Au/ZnO for the Semi-hydrogenation of Acetylene. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 40429-40440	9.5	1
9	First-principles study on the Cu-Au alloy monolayer supported on WC for hydrogen evolution. <i>Applied Surface Science</i> , 2021 , 565, 150568	6.7	1
8	Electronic and catalytic properties of Ti single atoms@SnO ₂ and its implications on sensing mechanism for CO. <i>Applied Surface Science</i> , 2022 , 594, 153500	6.7	1
7	Efficient capturing and oxidation of CO through bimetallic surface alloying on WC (0001). <i>Journal of Alloys and Compounds</i> , 2020 , 844, 156125	5.7	0
6	Efficient band structure engineering and visible-light response in SnS ₂ /GaS heterostructure by electric field and biaxial strain. <i>Superlattices and Microstructures</i> , 2019 , 134, 106210	2.8	0
5	Enhanced OER activity of FePc molecule by substrate effects: A first principles study. <i>Surface Science</i> , 2021 , 717, 122000	1.8	0
4	A variety of interface and strain tuning electronic properties of the MoS ₂ /Cr ₂ CX ₂ van der Waals heterostructures. <i>Journal Physics D: Applied Physics</i> , 2021 , 54, 345105	3	0
3	Surface vacancy on PtTe for promoting CO oxidation through efficiently activating O. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 025201	1.8	0
2	Structure and magnetic properties of CrN thin films on La _{0.67} Sr _{0.33} MnO ₃ . <i>Current Applied Physics</i> , 2018 , 18, 1320-1326	2.6	
1	A monolayer of Pd on ZrC(0 0 1) speeds up O ₂ dissociation: An ab initio study. <i>Applied Surface Science</i> , 2021 , 537, 148050	6.7	