Zongxian Yang

List of Publications by Year in Descending Order

209 papers	6,156 citations	42 h-index	70 g-index
212 ext. papers	7,032 ext. citations	4.9 avg, IF	6.27 L-index

#	Paper	IF	Citations
209	Ultrafast Kinetics in a PAN/MgFeO Flexible Free-Standing Anode Induced by Heterojunction and Oxygen Vacancies.. *ACS Applied Materials & Interfaces*, **2022**,	9.5	2
208	Electronic and catalytic properties of Ti single atoms@SnO2 and its implications on sensing mechanism for CO. *Applied Surface Science*, **2022**, 594, 153500	6.7	1
207	Enhanced OER activity of FePc molecule by substrate effects: A first principles study. *Surface Science*, **2021**, 717, 122000	1.8	0
206	Design of Highly Stable and Efficient Bifunctional MXene-Based Electrocatalysts for Oxygen Reduction and Evolution Reactions. *Physical Review Applied*, **2021**, 15,	4.3	2
205	A variety of interface and strain tuning electronic properties of the MoS2/Cr2CX 2 van der Waals heterostructures. *Journal Physics D: Applied Physics*, **2021**, 54, 345105	3	0
204	Design of promising single Rh atom catalyst for CO oxidation based on Graphdiyne sheets. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 130, 114676	3	11
203	A monolayer of Pd on ZrC(0 0 1) speeds up O2 dissociation: An ab initio study. *Applied Surface Science*, **2021**, 537, 148050	6.7	
202	Manipulation of electronic and magnetic properties of Cr2CX2 (X=F,O,OH) monolayer by applying mechanical strains. *Journal of Alloys and Compounds*, **2021**, 850, 156769	5.7	1
201	Substitution of Fe in hydroxyapatite as an efficient single-atom catalyst for oxygen reduction reaction in biofuel cells: A first-principles study. *Applied Surface Science*, **2021**, 539, 148233	6.7	1
200	Regulation of CO oxidation with Pd additives on Nb2CO2 MXene. *International Journal of Hydrogen Energy*, **2021**, 46, 8477-8485	6.7	2
199	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	13.1	28
198	Modulating oxygen electronic orbital occupancy of Cr-based MXenes via transition metal adsorbing for optimal HER activity. *International Journal of Hydrogen Energy*, **2021**, 46, 25457-25467	6.7	1
197	Au Species Boost the Catalytic Performance of Au/ZnO for the Semi-hydrogenation of Acetylene. *ACS Applied Materials & Interfaces*, **2021**, 13, 40429-40440	9.5	1
196	Cr2NX2 MXene (X = O, F, OH): A 2D ferromagnetic half-metal. *Applied Physics Letters*, **2021**, 119, 062404	3.4	6
195	First-principles study on the Cu-Au alloy monolayer supported on WC for hydrogen evolution. *Applied Surface Science*, **2021**, 565, 150568	6.7	1
194	Tuning the ORR activity of Pt-based TiCO MXenes by varying the atomic cluster size and doping with metals. *Nanoscale*, **2020**, 12, 12497-12507	7.7	12
193	Tailoring the Electronic Structure of Transition Metals by the VC MXene Support: Excellent Oxygen Reduction Performance Triggered by Metal-Support Interactions. *ACS Applied Materials & Interfaces*, **2020**, 12, 28206-28216	9.5	15

192	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	2.8	18
191	CO2 Reduction on Metal- and Nitrogen-Codoped Graphene: Balancing Activity and Selectivity via Coordination Engineering. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 6134-6141	8.3	15
190	CO2 thermoreduction to methanol on the MoS2 supported single Co atom catalyst: A DFT study. *Applied Surface Science*, **2020**, 528, 147047	6.7	20
189	Efficient capturing and oxidation of CO through bimetallic surface alloying on WC (0001). *Journal of Alloys and Compounds*, **2020**, 844, 156125	5.7	0
188	Identification of Efficient Single-Atom Catalysts Based on V2CO2 MXene by ab Initio Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 4090-4100	3.8	15
187	Efficient metal overlayer catalysts on the NbC monolayer for CO oxidation from first-principles screening. *Journal of Physics Condensed Matter*, **2020**, 32, 175201	1.8	2
186	Recent progress of MXenes as the support of catalysts for the CO oxidation and oxygen reduction reaction. *Chinese Chemical Letters*, **2020**, 31, 931-936	8.1	17
185	Mitigation of CO poisoning on functionalized palladium monolayer supported on titanium carbide. *Surface and Coatings Technology*, **2020**, 402, 125925	4.4	1
184	Cooperative Catalysis toward Oxygen Reduction Reaction under Dual Coordination Environments on Intrinsic AMnO -Type Perovskites via Regulating Stacking Configurations of Coordination Units. *Advanced Materials*, **2020**, 32, e2006145	24	10
183	Surface vacancy on PtTe for promoting CO oxidation through efficiently activating O. *Journal of Physics Condensed Matter*, **2020**, 32, 025201	1.8	0
182	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	2.3	4
181	Identification of High-Performance Single-Atom MXenes Catalysts for Low-Temperature CO Oxidation. *Advanced Theory and Simulations*, **2019**, 2, 1900006	3.5	15
180	Substrate effects on the in-plane ferroelectric polarization of two-dimensional SnTe. *Physical Review B*, **2019**, 99,	3.3	10
179	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	2.3	6
178	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	13	42
177	Au monolayer on WC(0001) with enhanced activity towards NO oxidation: A theoretical study. *Applied Surface Science*, **2019**, 481, 369-373	6.7	10
176	Efficient band structure engineering and visible-light response in SnS2/GaS heterostructure by electric field and biaxial strain. *Superlattices and Microstructures*, **2019**, 134, 106210	2.8	0
175	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	6.7	3

174	Low-temperature preferential oxidation of CO over Ag monolayer decorated MoC (MXene) for purifying H. *Journal of Physics Condensed Matter*, **2019**, 31, 215201	1.8	6
173	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. *Applied Surface Science*, **2019**, 479, 590-594	6.7	21
172	Cooperative activation effect on H2O adsorption in MnO□o catalyzed steam methane reforming. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 1357-1361	2.3	3
171	An electronic perturbation in TiC supported platinum monolayer catalyst for enhancing water-gas shift performance: DFT study. *Journal of Physics Condensed Matter*, **2019**, 31, 305201	1.8	5
170	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	6.7	7
169	WS2/BSe van der Waals type-II heterostructure as a promising water splitting photocatalyst. *Materials Research Express*, **2019**, 6, 035513	1.7	12
168	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	5.7	7
167	Repairing single and double atomic vacancies in a CN monolayer with CO or NO molecules: a first-principles study. *Physical Chemistry Chemical Physics*, **2018**, 20, 13517-13527	3.6	34
166	The adsorption and dissociation of O2 on Pd and Pt modified TaC (1 0 0) surface: A first principles study. *Applied Surface Science*, **2018**, 439, 845-851	6.7	6
165	First-principles study for the enhanced sulfur tolerance of Ni(1□1□1) surface alloyed with Pb. *Surface Science*, **2018**, 670, 68-71	1.8	3
164	Coexistence of Type-I and Type-II Weyl Points in the Weyl-Semimetal OsC2. *Journal of Physical Chemistry C*, **2018**, 122, 3533-3538	3.8	15
163	A Au monolayer on WC(0001) with unexpected high activity towards CO oxidation. *Nanoscale*, **2018**, 10, 4753-4760	7.7	12
162	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	8.9	5
161	Detection of gas molecules on single Mn adatom adsorbed graphyne: a DFT-D study. *Journal Physics D: Applied Physics*, **2018**, 51, 065109	3	34
160	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	3.8	6
159	Single Pd atomic catalyst on MoCO monolayer (MXene): unusual activity for CO oxidation by trimolecular Eley-Rideal mechanism. *Physical Chemistry Chemical Physics*, **2018**, 20, 3504-3513	3.6	56
158	Bifunctional CoNx embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. *Carbon*, **2018**, 130, 112-119	10.4	149
157	The mechanism of the high resistance to sulfur poisoning of the rhenium doped nickel/yttria-stabilized zirconia. *Applied Surface Science*, **2018**, 447, 561-568	6.7	6

156	C3N monolayers as promising candidates for NO2 sensors. *Sensors and Actuators B: Chemical*, **2018**, 266, 664-673	8.5	126
155	Density functional study on the high catalytic performance of single metal atoms on the NbC(001) surface. *Physical Chemistry Chemical Physics*, **2018**, 20, 10302-10310	3.6	2
154	The first principles study of the sulfur oxidation on Ni surface with H2O. *Journal of Alloys and Compounds*, **2018**, 741, 1183-1187	5.7	7
153	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	6.7	20
152	The possible magnetoelectric coupling induced by adsorption in SnTe films. *Applied Surface Science*, **2018**, 428, 89-93	6.7	5
151	Structure and magnetic properties of CrN thin films on La0.67Sr0.33MnO3. *Current Applied Physics*, **2018**, 18, 1320-1326	2.6	
150	First principles study of the gas sensing 2D GeTe: atomic, electronic and transport properties. *Journal Physics D: Applied Physics*, **2018**, 51, 345304	3	9
149	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	3.8	48
148	TiC and TiN supported platinum monolayer as high-performance catalysts for CO oxidation: A DFT study. *Journal of Chemical Physics*, **2018**, 149, 054705	3.9	7
147	Dopant segregation and CO adsorption on doped Fe3O4 (1 1 1) surfaces: A first-principle study. *Journal of Catalysis*, **2018**, 364, 291-296	7.3	18
146	Effects of rare-earth doping on the ionic conduction of CeO2 in solid oxide fuel cells. *Ceramics International*, **2018**, 44, 3707-3711	5.1	17
145	First-principles study of adsorption-induced magnetic properties of InSe monolayers. *Applied Surface Science*, **2018**, 436, 419-423	6.7	12
144	Tunable Electric Properties of Bilayer □GeTe with Different Interlayer Distances and External Electric Fields. *Nanoscale Research Letters*, **2018**, 13, 400	5	17
143	Engineering the activity of CoNx-graphene for hydrogen evolution. *International Journal of Hydrogen Energy*, **2018**, 43, 20573-20579	6.7	21
142	Strong metal-support interactions impart activity in the oxygen reduction reaction: Au monolayer on MoC (MXene). *Journal of Physics Condensed Matter*, **2018**, 30, 475201	1.8	18
141	Design of Efficient Catalysts for CO Oxidation on Titanium Carbide-Supported Platinum via Computational Study. *Journal of Physical Chemistry C*, **2018**, 122, 25974-25982	3.8	8
140	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	3.8	63
139	Cu-Cluster-Doped Monolayer MoCO (MXene) as an Electron Reservoir for Catalyzing a CO Oxidation Reaction. *ACS Applied Materials & Interfaces*, **2018**, 10, 32903-32912	9.5	38

138	TiC supported single-atom platinum catalyst for CO oxidation: A density functional theory study. *Applied Surface Science*, **2018**, 453, 159-165	6.7	14
137	Enhanced sulfur resistance of Ni(1 1 1) surface alloyed with Ge: A first principles study. *Surface Science*, **2018**, 677, 115-120	1.8	4
136	High resistance to sulfur poisoning of Ni with copper skin under electric field. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 671-678	2.3	1
135	A theoretical study of the lowest-energy PtPd co-doped silicon clusters: Chirality and fluxional transformation. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 873-878	2.3	1
134	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. *Carbon*, **2017**, 118, 35-42	10.4	126
133	A possible highly active supported Ni dimer catalyst for O2 dissociation: A first-principles study. *Applied Surface Science*, **2017**, 402, 168-174	6.7	4
132	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	3.6	13
131	A promising single atom catalyst for CO oxidation: Ag on boron vacancies of h-BN sheets. *Physical Chemistry Chemical Physics*, **2017**, 19, 16795-16805	3.6	84
130	Sulfur doped graphene as a promising metal-free electrocatalyst for oxygen reduction reaction: a DFT-D study. *RSC Advances*, **2017**, 7, 20398-20405	3.7	37
129	Efficient noble metal nanocatalysts supported on HfC(001) for O2 dissociation. *AIP Advances*, **2017**, 7, 035015	1.5	5
128	Electronic structure and optical properties for blue phosphorene/graphene-like GaN van der Waals heterostructures. *Current Applied Physics*, **2017**, 17, 1714-1720	2.6	21
127	First-principles investigation of HS adsorption and dissociation on titanium carbide surfaces. *Physical Chemistry Chemical Physics*, **2017**, 19, 27116-27122	3.6	3
126	Accelerating oxygen reduction on Pt monolayer via substrate compression. *Journal Physics D: Applied Physics*, **2017**, 50, 435501	3	1
125	Novel two-dimensional ferroelectric PbTe under tension: A first-principles prediction. *Journal of Applied Physics*, **2017**, 122, 064101	2.5	22
124	Density functional study on the resistance to sulfur poisoning of Pt (x = 0, 1, 4 and 8) modified □MoC(0001) surfaces. *Physical Chemistry Chemical Physics*, **2017**, 19, 24879-24885	3.6	1
123	Interaction between HO, N, CO, NO, NO and NO molecules and a defective WSe monolayer. *Physical Chemistry Chemical Physics*, **2017**, 19, 26022-26033	3.6	42
122	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	3.8	16
121	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. *Applied Surface Science*, **2017**, 426, 1232-1240	6.7	75

120	Effects of Sm doping content on the ionic conduction of CeO2 in SOFCs from first principles. *Applied Physics Letters*, **2017**, 111, 023903	3.4	16
119	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	6.7	11
118	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	3.8	7
117	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. *Applied Surface Science*, **2017**, 394, 47-57	6.7	9
116	Investigations on the origin of ferromagnetism of Cu doped anatase TiO 2 nanotubes. *Materials Research Bulletin*, **2017**, 86, 287-294	5.1	9
115	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	3.9	8
114	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	10	16
113	Tuning metal cluster catalytic activity with morphology and composition: a DFT study of O2 dissociation at the global minimum of PtmPdn (m + n = 5) clusters. *RSC Advances*, **2016**, 6, 104388-104397	3.7	18
112	The stability of TiC surfaces in the environment with various carbon chemical potential and surface defects. *Applied Surface Science*, **2016**, 386, 202-209	6.7	12
111	Repairing sulfur vacancies in the MoS2 monolayer by using CO, NO and NO2 molecules. *Journal of Materials Chemistry C*, **2016**, 4, 7093-7101	7.1	88
110	A first principles study of O2 dissociation on Pt modified ZrC(100) surface. *Chemical Physics Letters*, **2016**, 649, 141-147	2.5	10
109	Novel Ag@C nanocables supported Pd anodes and its implication in energy conversion using direct liquid fuel cells. *Applied Energy*, **2016**, 175, 429-434	10.7	13
108	A comparison study of oxygen reduction on the supported Pt, Pd, Au monolayer on WC(0001). *Journal of Power Sources*, **2016**, 321, 163-173	8.9	31
107	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	6.7	78
106	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		60
105	Modulating electronic, magnetic and chemical properties of MoS2 monolayer sheets by substitutional doping with transition metals. *Applied Surface Science*, **2016**, 364, 181-189	6.7	120
104	Intrinsic defect-mediated magnetism in Fe□ codoped TiO 2. *Journal of Alloys and Compounds*, **2016** , 657, 372-378	5.7	15
103	Investigations on the origin of ferromagnetism in Ga1□CrxN and Si-doped Ga1□CrxN films: Experiments and theory. *Journal of Alloys and Compounds*, **2016**, 658, 800-805	5.7	1

102	CO oxidation catalyzed by the single Co atom embedded hexagonal boron nitride nanosheet: a DFT-D study. *Physical Chemistry Chemical Physics*, **2016**, 18, 21865-70	3.6	81
101	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	3.9	17
100	Formaldehyde molecule adsorption on the doped monolayer MoS2: A first-principles study. *Applied Surface Science*, **2016**, 371, 180-188	6.7	99
99	3d transition metal embedded C2N monolayers as promising single-atom catalysts: A first-principles study. *Carbon*, **2016**, 105, 463-473	10.4	132
98	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	6.7	223
97	Effects of a TiC substrate on the catalytic activity of Pt for NO reduction. *Physical Chemistry Chemical Physics*, **2016**, 18, 13304-9	3.6	14
96	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	6.7	16
95	The mechanism of oxygen activation on single Pt-atom doped SnO2(110) surface. *Journal of Materials Science*, **2016**, 51, 10400-10407	4.3	24
94	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	6.7	39
93	Effects of Si-doping on magnetic properties of Ga1−xCrxN. *Journal of Magnetism and Magnetic Materials*, **2015**, 374, 564-568	2.8	2
92	Single Pt atom stabilized on nitrogen doped graphene: CO oxidation readily occurs via the tri-molecular Eley-Rideal mechanism. *Physical Chemistry Chemical Physics*, **2015**, 17, 20006-13	3.6	76
91	Growth mechanism and controllable synthesis of graphene on CuNi alloy surface in the initial growth stages. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2015**, 379, 1361-1365	2.3	11
90	Pd1/BN as a promising single atom catalyst of CO oxidation: a dispersion-corrected density functional theory study. *RSC Advances*, **2015**, 5, 84381-84388	3.7	56
89	Tuning the catalytic activity of AgPd alloy cluster for hydrogen dissociation by controlling the Pd ratio. *Computational and Theoretical Chemistry*, **2015**, 1071, 39-45	2	8
88	Hollow PdCu nanocubes supported by N-doped graphene: A surface science and electrochemical study. *International Journal of Hydrogen Energy*, **2015**, 40, 14305-14313	6.7	14
87	Adsorption and dissociation of ammonia on small iron clusters. *International Journal of Hydrogen Energy*, **2015**, 40, 346-352	6.7	15
86	Microstructure and magnetic properties of In1−xCrxN thin films. *Materials Science in Semiconductor Processing*, **2015**, 31, 147-152	4.3	3
85	The mechanisms of oxygen reduction reaction on phosphorus doped graphene: A first-principles study. *Journal of Power Sources*, **2015**, 276, 222-229	8.9	133

84	Interactions of small platinum clusters with the TiC(001) surface. *Journal of Applied Physics*, **2015**, 118, 185301	2.5	14
83	The sulfur poisoning of the nickel/oxygen-enriched yttria-stabilized zirconia. *Journal of Power Sources*, **2015**, 293, 635-641	8.9	9
82	Resistance to sulfur poisoning of Ni-based alloy with coinage (IB) metals. *Applied Surface Science*, **2015**, 357, 1785-1791	6.7	9
81	Understanding on the carbon deposition on the Nickel/Yttrium□Stabilized Zirconia anode caused by the CO containing fuels. *Journal of Power Sources*, **2015**, 279, 759-765	8.9	14
80	Effect of Cu doping on the catalytic activity of Fe3O4 in water-gas shift reactions. *International Journal of Hydrogen Energy*, **2015**, 40, 2193-2198	6.7	24
79	The origin of the low efficiency of carbon removal from the Nickel/Yttrium□Stabilized Zirconia triple-phase boundary by adsorbed water. *Journal of Power Sources*, **2015**, 279, 224-230	8.9	4
78	Novel catalytic activity for oxygen reduction reaction on MnN4 embedded graphene: A dispersion-corrected density functional theory study. *Carbon*, **2015**, 84, 500-508	10.4	147
77	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	2.3	15
76	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	8.9	15
75	The search for the good Pd-based catalyst for oxygen reduction reaction: core□shell M4@Pd20 nanowires. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	5
74	Ab initio atomistic thermodynamics study on the sulfur tolerance mechanism of the oxygen-enriched yttria-stabilized zirconia surface. *Surface Science*, **2014**, 622, 16-23	1.8	1
73	Depletion NO x Made Easy by Nitrogen Doped Graphene. *Catalysis Letters*, **2014**, 144, 1016-1022	2.8	16
72	Formation and catalytic activity of Pt supported on oxidized graphene for the CO oxidation reaction. *Physical Chemistry Chemical Physics*, **2014**, 16, 7887-95	3.6	73
71	Highly efficient Pd-based core-shell nanowire catalysts for O2 dissociation. *Physical Chemistry Chemical Physics*, **2014**, 16, 20532-6	3.6	5
70	A density function theory study on the NO reduction on nitrogen doped graphene. *Physical Chemistry Chemical Physics*, **2014**, 16, 20561-9	3.6	49
69	Several different charge transfer and Ce3+ localization scenarios for Rh□CeO2(111). *Journal of Materials Chemistry A*, **2014**, 2, 2333-2345	13	24
68	Resistance to sulfur poisoning of the gold doped nickel/yttria-stabilized zirconia with interface oxygen vacancy. *Journal of Power Sources*, **2014**, 271, 516-521	8.9	12
67	Sulfidation and Sulfur Recovery from SO2 over Ceria. *Journal of Physical Chemistry C*, **2014**, 118, 17499-17504	4.8	11

66	Direct CO oxidation by lattice oxygen on the SnO2(110) surface: a DFT study. *Physical Chemistry Chemical Physics*, **2014**, 16, 12488-94	3.6	40
65	Effects of substrate defects on the carbon cluster formation in graphene growth on Ni(111) surface. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 3055-3059	2.3	3
64	Importance of oxygen spillover for fuel oxidation on Ni/YSZ anodes in solid oxide fuel cells. *Physical Chemistry Chemical Physics*, **2014**, 16, 8536-40	3.6	12
63	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, 1033-40	3.6	13
62	Density functional theory study on the interaction of CO with the Fe3O4(001) surface. *Applied Surface Science*, **2014**, 317, 752-759	6.7	24
61	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	2.3	4
60	Theoretical study on the Si-doped graphene as an efficient metal-free catalyst for CO oxidation. *Applied Surface Science*, **2014**, 308, 402-407	6.7	100
59	Tuning the catalytic property of non-noble metallic impurities in graphene. *Carbon*, **2014**, 71, 139-149	10.4	78
58	The sulfur tolerance mechanism of the Cu/CeO2 system. *International Journal of Hydrogen Energy*, **2014**, 39, 1957-1966	6.7	5
57	The sensing mechanism of Pt-doped SnO2 surface toward CO: A first-principle study. *Sensors and Actuators B: Chemical*, **2014**, 202, 83-92	8.5	45
56	Theoretical study of the catalytic CO oxidation by Pt catalyst supported on Ge-doped grapheme. *Journal of Nanoscience and Nanotechnology*, **2014**, 14, 7117-24	1.3	19
55	O2 activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. *Applied Surface Science*, **2014**, 300, 91-97	6.7	8
54	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, 6626-8	5.8	21
53	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	2.3	15
52	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	8.9	24
51	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	8.9	9
50	Can H2S poison the surface of yttria-stabilized zirconia?. *International Journal of Hydrogen Energy*, **2013**, 38, 8974-8979	6.7	15
49	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	3.8	71

48	The formation and properties of Pt4 clusters on the defective graphene support. *Journal of Nanoscience and Nanotechnology*, **2013**, 13, 1612-5	1.3	5
47	The electronic structure and magnetism of KxFe2Se2. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 1072-1077	2.3	5
46	A theoretical simulation on the catalytic oxidation of CO on Pt/graphene. *Physical Chemistry Chemical Physics*, **2012**, 14, 16566-72	3.6	266
45	High Stability and Reactivity of Pt-Based Core‐Shell Nanoparticles for Oxygen Reduction Reaction. *Journal of Physical Chemistry C*, **2012**, 116, 13774-13780	3.8	17
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