

# Zhansheng Lu

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

125 papers	4,658 citations	40 h-index	64 g-index
127 ext. papers	5,566 ext. citations	5.5 avg, IF	5.92 L-index

#	Paper	IF	Citations
125	Dual-functional Z-scheme CdSe/Se/BiOBr photocatalyst: Generation of hydrogen peroxide and efficient degradation of ciprofloxacin. <i>Journal of Colloid and Interface Science</i> , <b>2022</b> , 606, 1715-1728	9.3	11
124	Electronic and catalytic properties of Ti single atoms@SnO <sub>2</sub> and its implications on sensing mechanism for CO. <i>Applied Surface Science</i> , <b>2022</b> , 594, 153500	6.7	1
123	Design of Highly Stable and Efficient Bifunctional MXene-Based Electrocatalysts for Oxygen Reduction and Evolution Reactions. <i>Physical Review Applied</i> , <b>2021</b> , 15,	4.3	2
122	Design of promising single Rh atom catalyst for CO oxidation based on Graphdiyne sheets. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 130, 114676	3	11
121	Introducing Crown Ether as a Functional Additive for High-Performance Dendrite-free Li Metal Batteries. <i>ACS Applied Energy Materials</i> , <b>2021</b> , 4, 7829-7838	6.1	3
120	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> , <b>2021</b> , 539, 148233	6.7	1
119	Enabling multifunctional electrocatalysts by modifying the basal plane of unifunctional 1TSMoS with anchored transition metal single atoms. <i>Nanoscale</i> , <b>2021</b> , 13, 13390-13400	7.7	16
118	Single-atom catalysts based on TiN for the electrocatalytic hydrogen evolution reaction: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 15685-15692	3.6	2
117	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> , <b>2021</b> , 11, 8929-8941	13.1	28
116	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 &amp; Interfaces</i> , <b>2020</b> , 12, 28206-28216	9.5	15
115	First-principles study of the oxygen reduction reaction on the boron-doped C <sub>9</sub> N <sub>4</sub> metal-free catalyst. <i>Applied Surface Science</i> , <b>2020</b> , 527, 146828	6.7	10
114	Construction of robust coupling interface between MoS <sub>2</sub> and nitrogen doped graphene for high performance sodium ion batteries. <i>Journal of Energy Chemistry</i> , <b>2020</b> , 48, 435-442	12	11
113	CO <sub>2</sub> thermoreduction to methanol on the MoS <sub>2</sub> supported single Co atom catalyst: A DFT study. <i>Applied Surface Science</i> , <b>2020</b> , 528, 147047	6.7	20
112	A Heterostructure Coupling of Bioinspired, Adhesive Polydopamine, and Porous Prussian Blue Nanocubics as Cathode for High-Performance Sodium-Ion Battery. <i>Small</i> , <b>2020</b> , 16, e1906946	11	23
111	Identification of Efficient Single-Atom Catalysts Based on V <sub>2</sub> CO <sub>2</sub> MXene by ab Initio Simulations. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 4090-4100	3.8	15
110	Facile one-pot synthesis of layered double hydroxides nanosheets with oxygen vacancies grown on carbon nanotubes for efficient oxygen evolution reaction. <i>Journal of Power Sources</i> , <b>2020</b> , 467, 228354	8.9	12
109	Three-Dimensional Superlithiophilic Interphase for Dendrite-Free Lithium Metal Anodes. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 5767-5774	9.5	20

108	Co-vacancy induced magneto-structural transformation in Co and Ge bidirectional-regulation MnCoGe systems. <i>Journal of Alloys and Compounds</i> , <b>2020</b> , 819, 153061	5.7	5
107	YS2 monolayer as a high-efficient anode material for rechargeable Li-ion and Na-ion batteries. <i>Solid State Ionics</i> , <b>2020</b> , 345, 115187	3.3	5
106	Chromium Single-Atom Catalyst with Graphyne Support: A Theoretical Study of NO Oxidation and Reduction. <i>ACS Catalysis</i> , <b>2020</b> , 10, 11951-11961	13.1	21
105	Transition metal embedded CN monolayers as promising catalysts for the hydrogen evolution reaction. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 20432-20441	3.6	18
104	Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	1
103	Novel structures of two-dimensional tungsten boride and their superconductivity. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 15327-15338	3.6	12
102	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> , <b>2019</b> , 7, 11400-11407 <sup>13</sup>		42
101	A sulfur coordination polymer with wide bandgap semiconductivity formed from zinc(II) and 5-methylsulfanyl-1,3,4-thiadiazole-2-thione. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2019</b> , 75, 1243-1249	0.8	2
100	Novel two-dimensional tetragonal vanadium carbides and nitrides as promising materials for Li-ion batteries. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 19513-19520	3.6	14
99	Microstructure, magnetic properties, and exchange bias in (Mn <sub>0.7</sub> Co <sub>0.3</sub> ) <sub>65</sub> Sn <sub>35</sub> alloy ribbons. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2019</b> , 492, 165686	2.8	3
98	Boron-doped InSe monolayer as a promising electrocatalyst for nitrogen reduction into ammonia at ambient conditions. <i>Applied Surface Science</i> , <b>2019</b> , 495, 143463	6.7	29
97	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. <i>Applied Surface Science</i> , <b>2019</b> , 479, 590-594	6.7	21
96	An electronic perturbation in TiC supported platinum monolayer catalyst for enhancing water-gas shift performance: DFT study. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 305201	1.8	5
95	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> , <b>2018</b> , 20, 13517-13527	3.6	34
94	Interaction of the O atom with the InSe monolayer: A first-principles study. <i>Vacuum</i> , <b>2018</b> , 153, 53-61	3.7	5
93	Detection of gas molecules on single Mn adatom adsorbed graphyne: a DFT-D study. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51, 065109	3	34
92	Bifunctional CoNx embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. <i>Carbon</i> , <b>2018</b> , 130, 112-119	10.4	149
91	C3N monolayers as promising candidates for NO <sub>2</sub> sensors. <i>Sensors and Actuators B: Chemical</i> , <b>2018</b> , 266, 664-673	8.5	126

90	The role of the intrinsic Se and In vacancies in the interaction of O <sub>2</sub> and H <sub>2</sub> O molecules with the InSe monolayer. <i>Applied Surface Science</i> , <b>2018</b> , 434, 215-227	6.7	20
89	Sodium storage mechanism of N, S co-doped nanoporous carbon: Experimental design and theoretical evaluation. <i>Energy Storage Materials</i> , <b>2018</b> , 11, 274-281	19.4	83
88	First-principles calculations of structural, electronic, magnetic and elastic properties of MoFeB under high pressure. <i>Royal Society Open Science</i> , <b>2018</b> , 5, 172247	3.3	2
87	Structure and magnetic properties of CrN thin films on La <sub>0.67</sub> Sr <sub>0.33</sub> MnO <sub>3</sub> . <i>Current Applied Physics</i> , <b>2018</b> , 18, 1320-1326	2.6	
86	Modulating the band structure and sub-bandgap absorption of Co-hyperdoped silicon by co-doping with shallow-level elements. <i>Applied Physics Express</i> , <b>2018</b> , 11, 061301	2.4	0
85	Boron-Doped C <sub>3</sub> N Monolayer as a Promising Metal-Free Oxygen Reduction Reaction Catalyst: A Theoretical Insight. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 20312-20322	3.8	48
84	Manganese-Doped CeO <sub>2</sub> Nanocubes for Catalytic Combustion of Chlorobenzene: An Experimental and Density Functional Theory Study. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2018</b> , 18, 3348-3355	1.3	6
83	Engineering the activity of CoN <sub>x</sub> -graphene for hydrogen evolution. <i>International Journal of Hydrogen Energy</i> , <b>2018</b> , 43, 20573-20579	6.7	21
82	First-Principles Study on the Single Ir Atom Embedded Graphdiyne: An Efficient Catalyst for CO Oxidation. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 23481-23492	3.8	63
81	B <sub>40</sub> and M@B <sub>40</sub> (MLi and Ba) fullerenes as potential molecular sensors for acetone detection: A first-principles study. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 264, 1-8	6	16
80	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> , <b>2017</b> , 381, 873-878	2.3	1
79	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. <i>Carbon</i> , <b>2017</b> , 118, 35-42	10.4	126
78	Mechanisms of direct hydrogen peroxide synthesis on silicon and phosphorus dual-doped graphene: a DFT-D study. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 9007-9015	3.6	13
77	A promising single atom catalyst for CO oxidation: Ag on boron vacancies of h-BN sheets. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 16795-16805	3.6	84
76	Sulfur doped graphene as a promising metal-free electrocatalyst for oxygen reduction reaction: a DFT-D study. <i>RSC Advances</i> , <b>2017</b> , 7, 20398-20405	3.7	37
75	Electronic structure and optical properties for blue phosphorene/graphene-like GaN van der Waals heterostructures. <i>Current Applied Physics</i> , <b>2017</b> , 17, 1714-1720	2.6	21
74	Accelerating oxygen reduction on Pt monolayer via substrate compression. <i>Journal Physics D: Applied Physics</i> , <b>2017</b> , 50, 435501	3	1
73	Interaction between HO, N, CO, NO, NO and NO molecules and a defective WSe monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 26022-26033	3.6	42

72	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. <i>Applied Surface Science</i> , <b>2017</b> , 426, 1232-1240	6.7	75
71	Tuning the Physical and Chemical Properties of 2D InSe with Interstitial Boron Doping: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 28312-28316	3.8	7
70	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. <i>Applied Surface Science</i> , <b>2017</b> , 394, 47-57	6.7	9
69	Tuning metal cluster catalytic activity with morphology and composition: a DFT study of O <sub>2</sub> dissociation at the global minimum of Pt <sub>m</sub> Pd <sub>n</sub> (m + n = 5) clusters. <i>RSC Advances</i> , <b>2016</b> , 6, 104388-104397	3.7	18
68	Repairing sulfur vacancies in the MoS <sub>2</sub> monolayer by using CO, NO and NO <sub>2</sub> molecules. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 7093-7101	7.1	88
67	A first principles study of O <sub>2</sub> dissociation on Pt modified ZrC(100) surface. <i>Chemical Physics Letters</i> , <b>2016</b> , 649, 141-147	2.5	10
66	A comparison study of oxygen reduction on the supported Pt, Pd, Au monolayer on WC(0001). <i>Journal of Power Sources</i> , <b>2016</b> , 321, 163-173	8.9	31
65	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> , <b>2016</b> , 360, 1-7	6.7	78
64	Single non-noble-metal cobalt atom stabilized by pyridinic vacancy graphene: An efficient catalyst for CO oxidation. <i>Journal of Molecular Catalysis A</i> , <b>2016</b> , 417, 28-35		60
63	Modulating electronic, magnetic and chemical properties of MoS <sub>2</sub> monolayer sheets by substitutional doping with transition metals. <i>Applied Surface Science</i> , <b>2016</b> , 364, 181-189	6.7	120
62	First-principles study of O <sub>2</sub> adsorption on Al-doped ZnO(1010) surface. <i>Sensors and Actuators B: Chemical</i> , <b>2016</b> , 224, 372-380	8.5	23
61	CO oxidation catalyzed by the single Co atom embedded hexagonal boron nitride nanosheet: a DFT-D study. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 21865-70	3.6	81
60	A facile post-process method to enhance crystallinity and electrochemical properties of SnO <sub>2</sub> /rGO composites with three-dimensional hierarchically porous structure. <i>RSC Advances</i> , <b>2016</b> , 6, 106275-106284	3.7	8
59	Formaldehyde molecule adsorption on the doped monolayer MoS <sub>2</sub> : A first-principles study. <i>Applied Surface Science</i> , <b>2016</b> , 371, 180-188	6.7	99
58	3d transition metal embedded C <sub>2</sub> N monolayers as promising single-atom catalysts: A first-principles study. <i>Carbon</i> , <b>2016</b> , 105, 463-473	10.4	132
57	The adsorption of CO and NO on the MoS <sub>2</sub> monolayer doped with Au, Pt, Pd, or Ni: A first-principles study. <i>Applied Surface Science</i> , <b>2016</b> , 383, 98-105	6.7	223
56	A theoretical understanding on the CO-tolerance mechanism of the WC(0001) supported Pt monolayer: Some improvement strategies. <i>Applied Surface Science</i> , <b>2016</b> , 389, 455-461	6.7	16
55	First-principles and experimental study of nitrogen/sulfur co-doped carbon nanosheets as anodes for rechargeable sodium ion batteries. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 15565-15574	13	104

54	The mechanism of oxygen activation on single Pt-atom doped SnO <sub>2</sub> (110) surface. <i>Journal of Materials Science</i> , <b>2016</b> , 51, 10400-10407	4.3	24
53	The mechanism of oxygen reduction reaction on CoN <sub>4</sub> embedded graphene: A combined kinetic and atomistic thermodynamic study. <i>International Journal of Hydrogen Energy</i> , <b>2016</b> , 41, 21212-21220	6.7	39
52	Coadsorption of gold with chlorine on CeO <sub>2</sub> (111) surfaces: A first principles study. <i>Chinese Physics B</i> , <b>2015</b> , 24, 026801	1.2	3
51	From the Surface Reaction Control to Gas-Diffusion Control: The Synthesis of Hierarchical Porous SnO <sub>2</sub> Microspheres and Their Gas-Sensing Mechanism. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 15963-15976	3.8	41
50	Adsorption and oxidation of NO on various SnO <sub>2</sub> (1 1 0) surfaces: A density functional theory study. <i>Sensors and Actuators B: Chemical</i> , <b>2015</b> , 221, 717-722	8.5	40
49	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> , <b>2015</b> , 17, 20006-13	3.6	76
48	Geometric stability and reaction activity of Pt clusters adsorbed graphene substrates for catalytic CO oxidation. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 11598-608	3.6	17
47	Pd <sub>1</sub> /BN as a promising single atom catalyst of CO oxidation: a dispersion-corrected density functional theory study. <i>RSC Advances</i> , <b>2015</b> , 5, 84381-84388	3.7	56
46	Graphyne as a promising substrate for the noble-metal single-atom catalysts. <i>Carbon</i> , <b>2015</b> , 95, 756-765	10.4	145
45	Adsorption of the water molecule on monolayer graphene surface has effect on its optical properties. <i>IOP Conference Series: Materials Science and Engineering</i> , <b>2015</b> , 87, 012101	0.4	2
44	CO catalytic oxidation on Al-doped graphene-like ZnO monolayer sheets: a first-principles study. <i>Journal of Materials Chemistry C</i> , <b>2015</b> , 3, 9964-9972	7.1	49
43	Adsorption and dissociation of ammonia on small iron clusters. <i>International Journal of Hydrogen Energy</i> , <b>2015</b> , 40, 346-352	6.7	15
42	CO catalytic oxidation on iron-embedded monolayer MoS <sub>2</sub> . <i>Applied Surface Science</i> , <b>2015</b> , 328, 71-77	6.7	84
41	The mechanisms of oxygen reduction reaction on phosphorus doped graphene: A first-principles study. <i>Journal of Power Sources</i> , <b>2015</b> , 276, 222-229	8.9	133
40	Novel catalytic activity for oxygen reduction reaction on MnN <sub>4</sub> embedded graphene: A dispersion-corrected density functional theory study. <i>Carbon</i> , <b>2015</b> , 84, 500-508	10.4	147
39	Depletion NO x Made Easy by Nitrogen Doped Graphene. <i>Catalysis Letters</i> , <b>2014</b> , 144, 1016-1022	2.8	16
38	Formation and catalytic activity of Pt supported on oxidized graphene for the CO oxidation reaction. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 7887-95	3.6	73
37	A density function theory study on the NO reduction on nitrogen doped graphene. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 20561-9	3.6	49



36	Several different charge transfer and Ce <sup>3+</sup> localization scenarios for Rh/CeO <sub>2</sub> (111). <i>Journal of Materials Chemistry A</i> , <b>2014</b> , 2, 2333-2345	13	24
35	Effect of lattice strain on the oxygen vacancy formation and hydrogen adsorption at CeO <sub>2</sub> (111) surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2014</b> , 378, 2570-2575	2.3	61
34	Sulfidation and Sulfur Recovery from SO <sub>2</sub> over Ceria. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 17499-17504	13.504	11
33	Direct CO oxidation by lattice oxygen on the SnO <sub>2</sub> (110) surface: a DFT study. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 12488-94	3.6	40
32	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> , <b>2014</b> , 378, 659-666	2.3	4
31	Theoretical study on the Si-doped graphene as an efficient metal-free catalyst for CO oxidation. <i>Applied Surface Science</i> , <b>2014</b> , 308, 402-407	6.7	100
30	Tuning the catalytic property of non-noble metallic impurities in graphene. <i>Carbon</i> , <b>2014</b> , 71, 139-149	10.4	78
29	The sulfur tolerance mechanism of the Cu/CeO <sub>2</sub> system. <i>International Journal of Hydrogen Energy</i> , <b>2014</b> , 39, 1957-1966	6.7	5
28	The sensing mechanism of Pt-doped SnO <sub>2</sub> surface toward CO: A first-principle study. <i>Sensors and Actuators B: Chemical</i> , <b>2014</b> , 202, 83-92	8.5	45
27	Theoretical study of the catalytic CO oxidation by Pt catalyst supported on Ge-doped grapheme. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2014</b> , 14, 7117-24	1.3	19
26	O <sub>2</sub> activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. <i>Applied Surface Science</i> , <b>2014</b> , 300, 91-97	6.7	8
25	Electric field effects on the excited properties of Si <sub>2</sub> N <sub>2</sub> molecule with special configuration:a density-functional study. <i>Wuli Xuebao/Acta Physica Sinica</i> , <b>2014</b> , 63, 103101	0.6	
24	Palladium nanoparticles with high energy facets as a key factor in dissociating O <sub>2</sub> in the solvent-free selective oxidation of alcohols. <i>Chemical Communications</i> , <b>2013</b> , 49, 6626-8	5.8	21
23	First-principles studies of Fe atoms adsorption on hydrogen-terminated boron nitride nanoribbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2013</b> , 377, 1016-1020	2.3	12
22	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> , <b>2013</b> , 237, 128-131	8.9	24
21	Can H <sub>2</sub> S poison the surface of yttria-stabilized zirconia?. <i>International Journal of Hydrogen Energy</i> , <b>2013</b> , 38, 8974-8979	6.7	15
20	A first-principle study on the interfacial properties of Cu/CeO <sub>2</sub> (110). <i>Wuli Xuebao/Acta Physica Sinica</i> , <b>2013</b> , 62, 117301	0.6	6
19	Sulfidation of Ceria Surfaces from Sulfur and Sulfur Diffusion. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 8417-8425	3.8	18

18	First-principles studies of BN sheets with absorbed transition metal single atoms or dimers: stabilities, electronic structures, and magnetic properties. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 145501	1.8	28
17	First principles study of the magnetism driven by cation defects in CeO <sub>2</sub> : the important role of O2p states. <i>Chinese Physics B</i> , <b>2012</b> , 21, 047505	1.2	8
16	Cu-doped ceria: Oxygen vacancy formation made easy. <i>Chemical Physics Letters</i> , <b>2011</b> , 510, 60-66	2.5	45
15	SOx on ceria from adsorbed SO <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 184703	3.9	30
14	Interfacial properties of NM/CeO <sub>2</sub> (111) (NM = noble metal atoms or clusters of Pd, Pt and Rh): a first principles study. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 475003	1.8	29
13	Physisorbed, Chemisorbed, and Oxidized CO on Highly Active Cu/CeO <sub>2</sub> (111). <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 4486-4494	3.8	99
12	Oxygen vacancy pairs on CeO <sub>2</sub> (110): A DFT + U study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2009</b> , 373, 2786-2792	2.3	37
11	Observation of rotated-oriented attachment during the growth of Ag <sub>2</sub> S nanorods under mediation of protein. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 9795-801	3.4	18
10	First-Principles Study on the Effects of Zr Dopant on the CO Adsorption on Ceria. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 15341-15347	3.8	26
9	Structural and electronic properties of NM-doped ceria (NM = Pt, Rh): a first-principles study. <i>Journal of Physics Condensed Matter</i> , <b>2008</b> , 20, 035210	1.8	36
8	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. <i>Surface Science</i> , <b>2008</b> , 602, 1199-1206	1.8	61
7	Interfacial properties of Ce <sub>0.75</sub> Zr <sub>0.25</sub> O <sub>2</sub> supported noble metals (Pd, Pt) from first principles. <i>European Physical Journal B</i> , <b>2008</b> , 63, 455-460	1.2	2
6	Oxygen vacancy formation energy at the Pd/CeO <sub>2</sub> (111) interface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2007</b> , 369, 132-139	2.3	63
5	Oxygen vacancy formation energy in Pd-doped ceria: a DFT+U study. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 074704	3.9	90
4	First-principles study of the Pt/CeO <sub>2</sub> (111) interface. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	73
3	Structure and analytical potential energy function for the ground state of the BC <sub>x</sub> (x=0, ∞). <i>Chinese Physics B</i> , <b>2006</b> , 15, 1257-1261		7
2	A polyoxometalate cluster-based single-atom catalyst for NH <sub>3</sub> synthesis via an enzymatic mechanism. <i>Journal of Materials Chemistry A</i> ,	13	4
1	An efficient screening strategy towards multifunctional catalysts for the simultaneous electroreduction of NO <sub>3</sub> <sup>-</sup> /NO <sub>2</sub> <sup>-</sup> and NO to NH <sub>3</sub> . <i>Journal of Materials Chemistry A</i> ,	13	8



