Zhansheng Lu

List of Publications by Citations

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	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
124	Bifunctional CoNx embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. *Carbon*, **2018**, 130, 112-119	10.4	149
123	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
122	Graphyne as a promising substrate for the noble-metal single-atom catalysts. *Carbon*, **2015**, 95, 756-765	10.4	145
121	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
120	3d transition metal embedded C2N monolayers as promising single-atom catalysts: A first-principles study. *Carbon*, **2016**, 105, 463-473	10.4	132
119	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. *Carbon*, **2017**, 118, 35-42	10.4	126
118	C3N monolayers as promising candidates for NO2 sensors. *Sensors and Actuators B: Chemical*, **2018**, 266, 664-673	8.5	126
117	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
116	First-principles and experimental study of nitrogen/sulfur co-doped carbon nanosheets as anodes for rechargeable sodium ion batteries. *Journal of Materials Chemistry A*, **2016**, 4, 15565-15574	13	104
115	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
114	Physisorbed, Chemisorbed, and Oxidized CO on Highly Active Cu□CeO2(111). *Journal of Physical Chemistry C*, **2010**, 114, 4486-4494	3.8	99
113	Formaldehyde molecule adsorption on the doped monolayer MoS2: A first-principles study. *Applied Surface Science*, **2016**, 371, 180-188	6.7	99
112	Oxygen vacancy formation energy in Pd-doped ceria: a DFT+U study. *Journal of Chemical Physics*, **2007**, 127, 074704	3.9	90
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 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
109	CO catalytic oxidation on iron-embedded monolayer MoS2. *Applied Surface Science*, **2015**, 328, 71-77	6.7	84

108	Sodium storage mechanism of N, S co-doped nanoporous carbon: Experimental design and theoretical evaluation. *Energy Storage Materials*, **2018**, 11, 274-281	19.4	83
107	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
106	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
105	Tuning the catalytic property of non-noble metallic impurities in graphene. *Carbon*, **2014**, 71, 139-149	10.4	78
104	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
103	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. *Applied Surface Science*, **2017**, 426, 1232-1240	6.7	75
102	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
101	First-principles study of the Pt□eO2(111) interface. *Physical Review B*, **2007**, 76,	3.3	73
100	Oxygen vacancy formation energy at the Pd/CeO2(111) interface. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2007**, 369, 132-139	2.3	63
99	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
98	Effect of lattice strain on the oxygen vacancy formation and hydrogen adsorption at CeO2(111) surface. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2570-2575	2.3	61
97	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. *Surface Science*, **2008**, 602, 1199-1206	1.8	61
96	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
95	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
94	CO catalytic oxidation on Al-doped graphene-like ZnO monolayer sheets: a first-principles study. *Journal of Materials Chemistry C*, **2015**, 3, 9964-9972	7.1	49
93	A density function theory study on the NO reduction on nitrogen doped graphene. *Physical Chemistry Chemical Physics*, **2014**, 16, 20561-9	3.6	49
92	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
91	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

90	Cu-doped ceria: Oxygen vacancy formation made easy. *Chemical Physics Letters*, **2011**, 510, 60-66	2.5	45
89	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
88	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
87	From the Surface Reaction Control to Gas-Diffusion Control: The Synthesis of Hierarchical Porous SnO2 Microspheres and Their Gas-Sensing Mechanism. *Journal of Physical Chemistry C*, **2015**, 119, 15963-15976	3.8	41
86	Adsorption and oxidation of NO on various SnO2(1 1 0) surfaces: A density functional theory study. *Sensors and Actuators B: Chemical*, **2015**, 221, 717-722	8.5	40
85	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
84	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
83	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
82	Oxygen vacancy pairs on CeO2(110): A DFT + U study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 2786-2792	2.3	37
81	Structural and electronic properties of NM-doped ceria (NM = Pt, Rh): a first-principles study. *Journal of Physics Condensed Matter*, **2008**, 20, 035210	1.8	36
80	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
79	Detection of gas molecules on single Mn adatom adsorbed graphyne: a DFT-D study. *Journal Physics D: Applied Physics*, **2018**, 51, 065109	3	34
78	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
77	SOx on ceria from adsorbed SO2. *Journal of Chemical Physics*, **2011**, 134, 184703	3.9	30
76	Boron-doped InSe monolayer as a promising electrocatalyst for nitrogen reduction into ammonia at ambient conditions. *Applied Surface Science*, **2019**, 495, 143463	6.7	29
75	Interfacial properties of NM/CeO(2)(111) (NM = noble metal atoms or clusters of Pd, Pt and Rh): a first principles study. *Journal of Physics Condensed Matter*, **2010**, 22, 475003	1.8	29
74	First-principles studies of BN sheets with absorbed transition metal single atoms or dimers: stabilities, electronic structures, and magnetic properties. *Journal of Physics Condensed Matter*, **2012**, 24, 145501	1.8	28
73	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

72	First-Principles Study on the Effects of Zr Dopant on the CO Adsorption on Ceria. *Journal of Physical Chemistry C*, **2008**, 112, 15341-15347	3.8	26
71	Several different charge transfer and Ce3+ localization scenarios for Rh□CeO2(111). *Journal of Materials Chemistry A*, **2014**, 2, 2333-2345	13	24
70	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
69	The mechanism of oxygen activation on single Pt-atom doped SnO2(110) surface. *Journal of Materials Science*, **2016**, 51, 10400-10407	4.3	24
68	A Heterostructure Coupling of Bioinspired, Adhesive Polydopamine, and Porous Prussian Blue Nanocubics as Cathode for High-Performance Sodium-Ion Battery. *Small*, **2020**, 16, e1906946	11	23
67	First-principles study of O2 adsorption on Al-doped ZnO(101□0) surface. *Sensors and Actuators B: Chemical*, **2016**, 224, 372-380	8.5	23
66	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
65	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
64	Chromium Single-Atom Catalyst with Graphyne Support: A Theoretical Study of NO Oxidation and Reduction. *ACS Catalysis*, **2020**, 10, 11951-11961	13.1	21
63	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. *Applied Surface Science*, **2019**, 479, 590-594	6.7	21
62	Engineering the activity of CoNx-graphene for hydrogen evolution. *International Journal of Hydrogen Energy*, **2018**, 43, 20573-20579	6.7	21
61	CO2 thermoreduction to methanol on the MoS2 supported single Co atom catalyst: A DFT study. *Applied Surface Science*, **2020**, 528, 147047	6.7	20
60	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
59	Three-Dimensional Superlithiophilic Interphase for Dendrite-Free Lithium Metal Anodes. *ACS Applied Materials & Interfaces*, **2020**, 12, 5767-5774	9.5	20
58	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
57	Transition metal embedded CN monolayers as promising catalysts for the hydrogen evolution reaction. *Physical Chemistry Chemical Physics*, **2019**, 21, 20432-20441	3.6	18
56	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
55	Sulfidation of Ceria Surfaces from Sulfur and Sulfur Diffusion. *Journal of Physical Chemistry C*, **2012**, 116, 8417-8425	3.8	18

54	Observation of rotated-oriented attachment during the growth of Ag2S nanorods under mediation of protein. *Journal of Physical Chemistry B*, **2008**, 112, 9795-801	3.4	18
53	Geometric stability and reaction activity of Pt clusters adsorbed graphene substrates for catalytic CO oxidation. *Physical Chemistry Chemical Physics*, **2015**, 17, 11598-608	3.6	17
52	Depletion NO x Made Easy by Nitrogen Doped Graphene. *Catalysis Letters*, **2014**, 144, 1016-1022	2.8	16
51	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
50	Enabling multifunctional electrocatalysts by modifying the basal plane of unifunctional 1TSMoS with anchored transition metal single atoms. *Nanoscale*, **2021**, 13, 13390-13400	7.7	16
49	B40 and M@B40 (MLi and Ba) fullerenes as potential molecular sensors for acetone detection: A first-principles study. *Journal of Molecular Liquids*, **2018**, 264, 1-8	6	16
48	Adsorption and dissociation of ammonia on small iron clusters. *International Journal of Hydrogen Energy*, **2015**, 40, 346-352	6.7	15
47	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
46	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
45	Can H2S poison the surface of yttria-stabilized zirconia?. *International Journal of Hydrogen Energy*, **2013**, 38, 8974-8979	6.7	15
44	Novel two-dimensional tetragonal vanadium carbides and nitrides as promising materials for Li-ion batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 19513-19520	3.6	14
43	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
42	Novel structures of two-dimensional tungsten boride and their superconductivity. *Physical Chemistry Chemical Physics*, **2019**, 21, 15327-15338	3.6	12
41	First-principles studies of Fe atoms adsorption on hydrogen-terminated boron nitride nanoribbons. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2013**, 377, 1016-1020	2.3	12
40	Facile one-pot synthesis of layered double hydroxides nanosheets with oxygen vacancies grown on carbon nanotubes for efficient oxygen evolution reaction. *Journal of Power Sources*, **2020**, 467, 228354	8.9	12
39	Construction of robust coupling interface between MoS2 and nitrogen doped graphene for high performance sodium ion batteries. *Journal of Energy Chemistry*, **2020**, 48, 435-442	12	11
38	Sulfidation and Sulfur Recovery from SO2 over Ceria. *Journal of Physical Chemistry C*, **2014**, 118, 17499-17504	3.3	11
37	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

36	Dual-functional Z-scheme CdSe/Se/BiOBr photocatalyst: Generation of hydrogen peroxide and efficient degradation of ciprofloxacin. *Journal of Colloid and Interface Science*, **2022**, 606, 1715-1728	9.3	11
35	First-principles study of the oxygen reduction reaction on the boron-doped C9N4 metal-free catalyst. *Applied Surface Science*, **2020**, 527, 146828	6.7	10
34	A first principles study of O2 dissociation on Pt modified ZrC(100) surface. *Chemical Physics Letters*, **2016**, 649, 141-147	2.5	10
33	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. *Applied Surface Science*, **2017**, 394, 47-57	6.7	9
32	O2 activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. *Applied Surface Science*, **2014**, 300, 91-97	6.7	8
31	First principles study of the magnetism driven by cation defects in CeO 2 : the important role of O2p states. *Chinese Physics B*, **2012**, 21, 047505	1.2	8
30	A facile post-process method to enhance crystallinity and electrochemical properties of SnO2/rGO composites with three-dimensional hierarchically porous structure. *RSC Advances*, **2016**, 6, 106275-106284	3.7	8
29	An efficient screening strategy towards multifunctional catalysts for the simultaneous electroreduction of NO3□NO2□and NO to NH3. *Journal of Materials Chemistry A*,	13	8
28	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
27	Structure and analytical potential energy function for the ground state of the BC x (x =0, □). *Chinese Physics B*, **2006**, 15, 1257-1261		7
26	Manganese-Doped CeO□Nanocubes for Catalytic Combustion of Chlorobenzene: An Experimental and Density Functional Theory Study. *Journal of Nanoscience and Nanotechnology*, **2018**, 18, 3348-3355	1.3	6
25	A first-principle study on the interfacial properties of Cu/CeO2(110). *Wuli Xuebao/Acta Physica Sinica*, **2013**, 62, 117301	0.6	6
24	Interaction of the O atom with the InSe monolayer: A first-principles study. *Vacuum*, **2018**, 153, 53-61	3.7	5
23	The sulfur tolerance mechanism of the Cu/CeO2 system. *International Journal of Hydrogen Energy*, **2014**, 39, 1957-1966	6.7	5
22	Co-vacancy induced magneto-structural transformation in Co and Ge bidirectional-regulation MnCoGe systems. *Journal of Alloys and Compounds*, **2020**, 819, 153061	5.7	5
21	YS2 monolayer as a high-efficient anode material for rechargeable Li-ion and Na-ion batteries. *Solid State Ionics*, **2020**, 345, 115187	3.3	5
20	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
19	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

18	A polyoxometalate cluster-based single-atom catalyst for NH3 synthesis via an enzymatic mechanism. *Journal of Materials Chemistry A*,	13	4
17	Coadsorption of gold with chlorine on CeO 2 (111) surfaces: A first principles study. *Chinese Physics B*, **2015**, 24, 026801	1.2	3
16	Microstructure, magnetic properties, and exchange bias in (Mn0.7Co0.3)65Sn35 alloy ribbons. *Journal of Magnetism and Magnetic Materials*, **2019**, 492, 165686	2.8	3
15	Introducing Crown Ether as a Functional Additive for High-Performance Dendrite-free Li Metal Batteries. *ACS Applied Energy Materials*, **2021**, 4, 7829-7838	6.1	3
14	Adsorption of the water molecule on monolayer graphene surface has effect on its optical properties. *IOP Conference Series: Materials Science and Engineering*, **2015**, 87, 012101	0.4	2
13	First-principles calculations of structural, electronic, magnetic and elastic properties of MoFeB under high pressure. *Royal Society Open Science*, **2018**, 5, 172247	3.3	2
12	A sulfur coordination polymer with wide bandgap semiconductivity formed from zinc(II) and 5-methylsulfanyl-1,3,4-thiadiazole-2-thione. *Acta Crystallographica Section C, Structural Chemistry*, **2019**, 75, 1243-1249	0.8	2
11	Interfacial properties of Ce0.75Zr0.25O2 supported noble metals (Pd, Pt) from first principles. *European Physical Journal B*, **2008**, 63, 455-460	1.2	2
10	Design of Highly Stable and Efficient Bifunctional MXene-Based Electrocatalysts for Oxygen Reduction and Evolution Reactions. *Physical Review Applied*, **2021**, 15,	4.3	2
9	Single-atom catalysts based on TiN for the electrocatalytic hydrogen evolution reaction: a theoretical study. *Physical Chemistry Chemical Physics*, **2021**, 23, 15685-15692	3.6	2
8	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
7	Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. *Nanomaterials*, **2019**, 9,	5.4	1
6	Accelerating oxygen reduction on Pt monolayer via substrate compression. *Journal Physics D: Applied Physics*, **2017**, 50, 435501	3	1
5	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
4	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
3	Modulating the band structure and sub-bandgap absorption of Co-hyperdoped silicon by co-doping with shallow-level elements. *Applied Physics Express*, **2018**, 11, 061301	2.4	0
2	Structure and magnetic properties of CrN thin films on La0.67Sr0.33MnO3. *Current Applied Physics*, **2018**, 18, 1320-1326	2.6	
1	Electric field effects on the excited properties of Si2N2 molecule with special configuration:a density-functional study. *Wuli Xuebao/Acta Physica Sinica*, **2014**, 63, 103101	0.6	