Zhansheng Lu

List of Publications by Year
in descending order

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127	6,323	46918	74018
papers	citations	47 h-index	75 g-index

127	127	127	5901
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The adsorption of CO and NO on the MoS2 monolayer doped with Au, Pt, Pd, or Ni: A first-principles study. Applied Surface Science, 2016, 383, 98-105.	3.1	321
2	Bifunctional CoNx embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. Carbon, 2018, 130, 112-119.	5.4	209
3	Graphyne as a promising substrate for the noble-metal single-atom catalysts. Carbon, 2015, 95, 756-765.	5.4	181
4	C3N monolayers as promising candidates for NO2 sensors. Sensors and Actuators B: Chemical, 2018, 266, 664-673.	4.0	172
5	3d transition metal embedded C2N monolayers as promising single-atom catalysts: A first-principles study. Carbon, 2016, 105, 463-473.	5.4	167
6	Novel catalytic activity for oxygen reduction reaction on MnN4 embedded graphene: A dispersion-corrected density functional theory study. Carbon, 2015, 84, 500-508.	5.4	166
7	The mechanisms of oxygen reduction reaction on phosphorus doped graphene: A first-principles study. Journal of Power Sources, 2015, 276, 222-229.	4.0	165
8	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. Carbon, 2017, 118, 35-42.	5.4	164
9	Modulating electronic, magnetic and chemical properties of MoS2 monolayer sheets by substitutional doping with transition metals. Applied Surface Science, 2016, 364, 181-189.	3.1	161
10	Formaldehyde molecule adsorption on the doped monolayer MoS2: A first-principles study. Applied Surface Science, 2016, 371, 180-188.	3.1	129
11	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.	5.2	128
12	Theoretical Inspection of M₁/PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). ACS Catalysis, 2021, 11, 8929-8941.	5.5	121
13	Theoretical study on the Si-doped graphene as an efficient metal-free catalyst for CO oxidation. Applied Surface Science, 2014, 308, 402-407.	3.1	115
14	Sodium storage mechanism of N, S co-doped nanoporous carbon: Experimental design and theoretical evaluation. Energy Storage Materials, 2018, 11, 274-281.	9.5	112
15	Repairing sulfur vacancies in the MoS₂ monolayer by using CO, NO and NO₂ molecules. Journal of Materials Chemistry C, 2016, 4, 7093-7101.	2.7	111
16	Physisorbed, Chemisorbed, and Oxidized CO on Highly Active Cuâ˜'CeO₂(111). Journal of Physical Chemistry C, 2010, 114, 4486-4494.	1.5	110
17	Oxygen vacancy formation energy in Pd-doped ceria: A DFT+U study. Journal of Chemical Physics, 2007, 127, 074704.	1.2	105
18	A promising single atom catalyst for CO oxidation: Ag on boron vacancies of h-BN sheets. Physical Chemistry Chemical Physics, 2017, 19, 16795-16805.	1.3	102

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19	CO catalytic oxidation on iron-embedded monolayer MoS2. Applied Surface Science, 2015, 328, 71-77.	3.1	100
20	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. Applied Surface Science, 2017, 426, 1232-1240.	3.1	99
21	CO oxidation catalyzed by the single Co atom embedded hexagonal boron nitride nanosheet: a DFT-D study. Physical Chemistry Chemical Physics, 2016, 18, 21865-21870.	1.3	96
22	Single Pt atom stabilized on nitrogen doped graphene: CO oxidation readily occurs via the tri-molecular Eleyâ€“Rideal mechanism. Physical Chemistry Chemical Physics, 2015, 17, 20006-20013.	1.3	91
23	First principles study on the interfacial properties of NM/graphdiyne (NM = Pd, Pt, Rh and Ir): The implications for NM growing. Applied Surface Science, 2016, 360, 1-7.	3.1	90
24	First-Principles Study on the Single Ir Atom Embedded Graphdiyne: An Efficient Catalyst for CO Oxidation. Journal of Physical Chemistry C, 2018, 122, 23481-23492.	1.5	87
25	Tuning the catalytic property of non-noble metallic impurities in graphene. Carbon, 2014, 71, 139-149.	5.4	85
26	First-principles study of thePtâˆ•CeO2(111)interface. Physical Review B, 2007, 76, .	1.1	82
27	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.	0.9	82
28	Boron-Doped C₃N Monolayer as a Promising Metal-Free Oxygen Reduction Reaction Catalyst: A Theoretical Insight. Journal of Physical Chemistry C, 2018, 122, 20312-20322.	1.5	78
29	Formation and catalytic activity of Pt supported on oxidized graphene for the CO oxidation reaction. Physical Chemistry Chemical Physics, 2014, 16, 7887-7895.	1.3	75
30	Oxygen vacancy formation energy at the Pd/CeO2(111) interface. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 369, 132-139.	0.9	70
31	Enabling multifunctional electrocatalysts by modifying the basal plane of unifunctional 1Tâ€²-MoS₂ with anchored transition metal single atoms. Nanoscale, 2021, 13, 13390-13400.	2.8	69
32	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. Surface Science, 2008, 602, 1199-1206.	0.8	68
33	Pd₁/BN as a promising single atom catalyst of CO oxidation: a dispersion-corrected density functional theory study. RSC Advances, 2015, 5, 84381-84388.	1.7	68
34	Single non-noble-metal cobalt atom stabilized by pyridinic vacancy graphene: An efficient catalyst for CO oxidation. Journal of Molecular Catalysis A, 2016, 417, 28-35.	4.8	68
35	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.	1.5	66
36	3D well-ordered porous phosphorus doped carbon as an anode for sodium storage: structure design, experimental and computational insights. Journal of Materials Chemistry A, 2019, 7, 11400-11407.	5.2	64

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37	Interaction between H₂O, N₂, CO, NO, NO₂ and N₂O molecules and a defective WSe₂ monolayer. Physical Chemistry Chemical Physics, 2017, 19, 26022-26033.	1.3	60
38	CO catalytic oxidation on Al-doped graphene-like ZnO monolayer sheets: a first-principles study. Journal of Materials Chemistry C, 2015, 3, 9964-9972.	2.7	58
39	A Heterostructure Coupling of Bioinspired, Adhesive Polydopamine, and Porous Prussian Blue Nanocubics as Cathode for Highâ€Performance Sodiumâ€Ion Battery. Small, 2020, 16, e1906946.	5.2	57
40	Detection of gas molecules on single Mn adatom adsorbed graphyne: a DFT-D study. Journal Physics D: Applied Physics, 2018, 51, 065109.	1.3	56
41	The sensing mechanism of Pt-doped SnO2 surface toward CO: A first-principle study. Sensors and Actuators B: Chemical, 2014, 202, 83-92.	4.0	55
42	Cu-doped ceria: Oxygen vacancy formation made easy. Chemical Physics Letters, 2011, 510, 60-66.	1.2	53
43	A density function theory study on the NO reduction on nitrogen doped graphene. Physical Chemistry Chemical Physics, 2014, 16, 20561-20569.	1.3	53
44	Sulfur doped graphene as a promising metal-free electrocatalyst for oxygen reduction reaction: a DFT-D study. RSC Advances, 2017, 7, 20398-20405.	1.7	53
45	An efficient screening strategy towards multifunctional catalysts for the simultaneous electroreduction of NO₃^â, NO₂^â and NO to NH₃. Journal of Materials Chemistry A, 2022, 10, 9707-9716.	5.2	52
46	Direct CO oxidation by lattice oxygen on the SnO₂(110) surface: a DFT study. Physical Chemistry Chemical Physics, 2014, 16, 12488-12494.	1.3	51
47	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.	4.0	51
48	The mechanism of oxygen reduction reaction on CoN4 embedded graphene: A combined kinetic and atomistic thermodynamic study. International Journal of Hydrogen Energy, 2016, 41, 21212-21220.	3.8	51
49	Chromium Single-Atom Catalyst with Graphyne Support: A Theoretical Study of NO Oxidation and Reduction. ACS Catalysis, 2020, 10, 11951-11961.	5.5	49
50	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.	5.0	47
51	Boron-doped InSe monolayer as a promising electrocatalyst for nitrogen reduction into ammonia at ambient conditions. Applied Surface Science, 2019, 495, 143463.	3.1	46
52	CO2 thermoreduction to methanol on the MoS2 supported single Co atom catalyst: A DFT study. Applied Surface Science, 2020, 528, 147047.	3.1	46
53	Oxygen vacancy pairs on CeO2(110): A DFT+U study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 2786-2792.	0.9	44
54	Repairing single and double atomic vacancies in a C₃N monolayer with CO or NO molecules: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 13517-13527.	1.3	41

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55	Structural and electronic properties of NM-doped ceria (NM = Pt, Rh): a first-principles study. Journal of Physics Condensed Matter, 2008, 20, 035210.	0.7	39
56	Tailoring the Electronic Structure of Transition Metals by the V₂C MXene Support: Excellent Oxygen Reduction Performance Triggered by Metalâ€“Support Interactions. ACS Applied Materials & Interfaces, 2020, 12, 28206-28216.	4.0	39
57	Three-Dimensional Superlithiophilic Interphase for Dendrite-Free Lithium Metal Anodes. ACS Applied Materials & Interfaces, 2020, 12, 5767-5774.	4.0	36
58	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.	4.0	35
59	Interfacial properties of NM/CeO₂(111) (NM = noble metal atoms or clusters of Pd, Pt and) Tj ETQq1 1 0.784314 rgBT /Ov	0.7	34
60	A comparison study of oxygen reduction on the supported Pt, Pd, Au monolayer on WC(0001). Journal of Power Sources, 2016, 321, 163-173.	4.0	34
61	Electronic structure and optical properties for blue phosphorene/graphene-like GaN van der Waals heterostructures. Current Applied Physics, 2017, 17, 1714-1720.	1.1	34
62	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.	0.7	33
63	SOx on ceria from adsorbed SO2. Journal of Chemical Physics, 2011, 134, 184703.	1.2	32
64	The mechanism of oxygen activation on single Pt-atom doped SnO2(110) surface. Journal of Materials Science, 2016, 51, 10400-10407.	1.7	32
65	Transition metal embedded C₃N monolayers as promising catalysts for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2019, 21, 20432-20441.	1.3	32
66	Identification of Efficient Single-Atom Catalysts Based on V₂CO₂ MXene by ab Initio Simulations. Journal of Physical Chemistry C, 2020, 124, 4090-4100.	1.5	31
67	Engineering the activity of CoNx-graphene for hydrogen evolution. International Journal of Hydrogen Energy, 2018, 43, 20573-20579.	3.8	29
68	First-Principles Study on the Effects of Zr Dopant on the CO Adsorption on Ceria. Journal of Physical Chemistry C, 2008, 112, 15341-15347.	1.5	27
69	The role of the intrinsic Se and In vacancies in the interaction of O2 and H2O molecules with the InSe monolayer. Applied Surface Science, 2018, 434, 215-227.	3.1	27
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.	4.0	26
71	Several different charge transfer and Ce³⁺localization scenarios for Rhâ€“CeO₂(111). Journal of Materials Chemistry A, 2014, 2, 2333-2345.	5.2	26
72	B40 and M@B40 (M Li and Ba) fullerenes as potential molecular sensors for acetone detection: A first-principles study. Journal of Molecular Liquids, 2018, 264, 1-8.	2.3	26

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73	Novel two-dimensional tetragonal vanadium carbides and nitrides as promising materials for Li-ion batteries. Physical Chemistry Chemical Physics, 2019, 21, 19513-19520.	1.3	26
74	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. Applied Surface Science, 2019, 479, 590-594.	3.1	26
75	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.	7.1	26
76	Palladium nanoparticles with high energy facets as a key factor in dissociating O2 in the solvent-free selective oxidation of alcohols. Chemical Communications, 2013, 49, 6626.	2.2	25
77	First-principles study of O2 adsorption on Al-doped ZnO(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 602 Td (xmlns:mml surface. Sensors and Actuators B: Chemical, 2016, 224, 372-380.	4.0	25
78	Observation of Rotated-Oriented Attachment during the Growth of Ag₂S Nanorods under Mediation of Protein. Journal of Physical Chemistry B, 2008, 112, 9795-9801.	1.2	23
79	Adsorption and dissociation of ammonia on small iron clusters. International Journal of Hydrogen Energy, 2015, 40, 346-352.	3.8	23
80	Novel structures of two-dimensional tungsten boride and their superconductivity. Physical Chemistry Chemical Physics, 2019, 21, 15327-15338.	1.3	23
81	A polyoxometalate cluster-based single-atom catalyst for NH₃ synthesis <i>via</i> an enzymatic mechanism. Journal of Materials Chemistry A, 2022, 10, 6165-6177.	5.2	23
82	A theoretical understanding on the CO-tolerance mechanism of the WC(0001) supported Pt monolayer: Some improvement strategies. Applied Surface Science, 2016, 389, 455-461.	3.1	22
83	Geometric stability and reaction activity of Pt clusters adsorbed graphene substrates for catalytic CO oxidation. Physical Chemistry Chemical Physics, 2015, 17, 11598-11608.	1.3	20
84	Sulfidation of Ceria Surfaces from Sulfur and Sulfur Diffusion. Journal of Physical Chemistry C, 2012, 116, 8417-8425.	1.5	19
85	Theoretical Study of the Catalytic CO Oxidation by Pt Catalyst Supported on Ge-Doped Graphene. Journal of Nanoscience and Nanotechnology, 2014, 14, 7117-7124.	0.9	19
86	Tuning metal cluster catalytic activity with morphology and composition: a DFT study of O₂ dissociation at the global minimum of Pt_mPd_n (m + n = 5) clusters. RSC Advances, 2016, 6, 104388-104397.	1.7	19
87	YS2 monolayer as a high-efficient anode material for rechargeable Li-ion and Na-ion batteries. Solid State Ionics, 2020, 345, 115187.	1.3	19
88	Mechanisms of direct hydrogen peroxide synthesis on silicon and phosphorus dual-doped graphene: a DFT-D study. Physical Chemistry Chemical Physics, 2017, 19, 9007-9015.	1.3	18
89	Design of promising single Rh atom catalyst for CO oxidation based on Graphdiyne sheets. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 130, 114676.	1.3	18
90	Can H2S poison the surface of yttria-stabilized zirconia?. International Journal of Hydrogen Energy, 2013, 38, 8974-8979.	3.8	16

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91	Depletion NO x Made Easy by Nitrogen Doped Graphene. Catalysis Letters, 2014, 144, 1016-1022.	1.4	16
92	First-principles study of the oxygen reduction reaction on the boron-doped C9N4 metal-free catalyst. Applied Surface Science, 2020, 527, 146828.	3.1	16
93	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.	0.9	14
94	CO oxidation on MXene (Mo2CS2) supported single-atom catalyst: A termolecular Eley-Rideal mechanism. Chinese Chemical Letters, 2023, 34, 107412.	4.8	13
95	O2 activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. Applied Surface Science, 2014, 300, 91-97.	3.1	11
96	Sulfidation and Sulfur Recovery from SO₂ over Ceria. Journal of Physical Chemistry C, 2014, 118, 17499-17504.	1.5	11
97	A first principles study of O2 dissociation on Pt modified ZrC(100) surface. Chemical Physics Letters, 2016, 649, 141-147.	1.2	11
98	Tuning the Physical and Chemical Properties of 2D InSe with Interstitial Boron Doping: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 28312-28316.	1.5	11
99	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. Applied Surface Science, 2017, 394, 47-57.	3.1	11
100	Design of Highly Stable and Efficient Bifunctional MX ene-Based Electrocatalysts for Oxygen Reduction and Evolution Reactions. Physical Review Applied, 2021, 15, .	1.5	11
101	Introducing Crown Ether as a Functional Additive for High-Performance Dendrite-free Li Metal Batteries. ACS Applied Energy Materials, 2021, 4, 7829-7838.	2.5	11
102	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.	1.7	9
103	First principles study of the magnetism driven by cation defects in CeO₂: the important role of O2p states. Chinese Physics B, 2012, 21, 047505.	0.7	8
104	An electronic perturbation in TiC supported platinum monolayer catalyst for enhancing waterâ€“gas shift performance: DFT study. Journal of Physics Condensed Matter, 2019, 31, 305201.	0.7	8
105	Co-vacancy induced magneto-structural transformation in Co and Ge bidirectional-regulation MnCoGe systems. Journal of Alloys and Compounds, 2020, 819, 153061.	2.8	8
106	Structure and analytical potential energy function for the ground state of the BC x (x =0, â€“1). Chinese Physics B, 2006, 15, 1257-1261.	1.3	7
107	First-principles calculations of structural, electronic, magnetic and elastic properties of Mo₂FeB₂under high pressure. Royal Society Open Science, 2018, 5, 172247.	1.1	7
108	Manganese-Doped CeO₂ Nanocubes for Catalytic Combustion of Chlorobenzene: An Experimental and Density Functional Theory Study. Journal of Nanoscience and Nanotechnology, 2018, 18, 3348-3355.	0.9	7

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109	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.	3.1	7
110	A first-principle study on the interfacial properties of Cu/CeO2(110). Wuli Xuebao/Acta Physica Sinica, 2013, 62, 117301.	0.2	7
111	Interaction of the O atom with the InSe monolayer: A first-principles study. Vacuum, 2018, 153, 53-61.	1.6	6
112	Single-atom catalysts based on TiN for the electrocatalytic hydrogen evolution reaction: a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 15685-15692.	1.3	6
113	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.	0.9	5
114	The sulfur tolerance mechanism of the Cu/CeO2 system. International Journal of Hydrogen Energy, 2014, 39, 1957-1966.	3.8	5
115	Intercalation assisted liquid phase production of disulfide zirconium nanosheets for efficient electrocatalytic dinitrogen reduction to ammonia. Green Energy and Environment, 2023, 8, 1174-1184.	4.7	5
116	Electronic and catalytic properties of Ti single atoms@SnO2 and its implications on sensing mechanism for CO. Applied Surface Science, 2022, 594, 153500.	3.1	5
117	Interfacial properties of Ce0.75Zr0.25O2 supported noble metals (Pd, Pt) from first principles. European Physical Journal B, 2008, 63, 455-460.	0.6	4
118	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.	0.3	4
119	Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. Nanomaterials, 2019, 9, 1420.	1.9	4
120	Coadsorption of gold with chlorine on CeO ₂ (111) surfaces: A first principles study. Chinese Physics B, 2015, 24, 026801.	0.7	3
121	Accelerating oxygen reduction on Pt monolayer via substrate compression. Journal Physics D: Applied Physics, 2017, 50, 435501.	1.3	3
122	Microstructure, magnetic properties, and exchange bias in (Mn0.7Co0.3)65Sn35 alloy ribbons. Journal of Magnetism and Magnetic Materials, 2019, 492, 165686.	1.0	3
123	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.	0.2	2
124	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.	0.9	1
125	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.	1.1	1
126	Structure and magnetic properties of CrN thin films on La0.67Sr0.33MnO3. Current Applied Physics, 2018, 18, 1320-1326.	1.1	0

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127	Electric field effects on the excited properties of Si2N2 molecule with special configurationï¼ša density-functional study. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 103101.	0.2	0