Zhansheng Lu

List of Publications by Year
in descending order

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127 papers	6,323 citations	46918 47 h-index	74018 75 g-index
127 all docs	127 docs citations	127 times ranked	5901 citing authors

#	Article	IF	Citations
1	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
2	CO oxidation on MXene (Mo2CS2) supported single-atom catalyst: A termolecular Eley-Rideal mechanism. Chinese Chemical Letters, 2023, 34, 107412.	4.8	13
3	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
4	A polyoxometalate cluster-based single-atom catalyst for NH₃ synthesis via an enzymatic mechanism. Journal of Materials Chemistry A, 2022, 10, 6165-6177.	5.2	23
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	Three-Dimensional Superlithiophilic Interphase for Dendrite-Free Lithium Metal Anodes. ACS Applied Materials & Interfaces, 2020, 12, 5767-5774.	4.0	36
15	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
16	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
17	Chromium Single-Atom Catalyst with Graphyne Support: A Theoretical Study of NO Oxidation and Reduction. ACS Catalysis, 2020, 10, 11951-11961.	5.5	49
18	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

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19	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
20	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
21	CO2 thermoreduction to methanol on the MoS2 supported single Co atom catalyst: A DFT study. Applied Surface Science, 2020, 528, 147047.	3.1	46
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	Transition metal embedded C₃N monolayers as promising catalysts for the hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2019, 21, 20432-20441.	1.3	32
30	Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. Nanomaterials, 2019, 9, 1420.	1.9	4
31	Novel structures of two-dimensional tungsten boride and their superconductivity. Physical Chemistry Chemical Physics, 2019, 21, 15327-15338.	1.3	23
32	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
33	Phosphorene: A promising metal free cathode material for proton exchange membrane fuel cell. Applied Surface Science, 2019, 479, 590-594.	3.1	26
34	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
35	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
36	Interaction of the O atom with the InSe monolayer: A first-principles study. Vacuum, 2018, 153, 53-61.	1.6	6

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37	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
38	Bifunctional CoNx embedded graphene electrocatalysts for OER and ORR: A theoretical evaluation. Carbon, 2018, 130, 112-119.	5.4	209
39	C3N monolayers as promising candidates for NO2 sensors. Sensors and Actuators B: Chemical, 2018, 266, 664-673.	4.0	172
40	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
41	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
42	Engineering the activity of CoNx-graphene for hydrogen evolution. International Journal of Hydrogen Energy, 2018, 43, 20573-20579.	3.8	29
43	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
44	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
45	First-principles calculations of structural, electronic, magnetic and elastic properties of Mo₂FeB₂under high pressure. Royal Society Open Science, 2018, 5, 172247.	1.1	7
46	Structure and magnetic properties of CrN thin films on La0.67Sr0.33MnO3. Current Applied Physics, 2018, 18, 1320-1326.	1.1	0
47	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
48	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
49	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
50	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
51	CO oxidation on single Pd atom embedded defect-graphene via a new termolecular Eley-Rideal mechanism. Carbon, 2017, 118, 35-42.	5.4	164
52	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
53	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
54	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

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55	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
56	Accelerating oxygen reduction on Pt monolayer via substrate compression. Journal Physics D: Applied Physics, 2017, 50, 435501.	1.3	3
57	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
58	CO oxidation on Mn-N4 porphyrin-like carbon nanotube: A DFT-D study. Applied Surface Science, 2017, 426, 1232-1240.	3.1	99
59	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
60	Platinum adsorption on ceria: A comparative theoretical study of different surfaces. Applied Surface Science, 2017, 394, 47-57.	3.1	11
61	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
62	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
63	Formaldehyde molecule adsorption on the doped monolayer MoS2: A first-principles study. Applied Surface Science, 2016, 371, 180-188.	3.1	129
64	3d transition metal embedded C2N monolayers as promising single-atom catalysts: A first-principles study. Carbon, 2016, 105, 463-473.	5.4	167
65	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
66	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
67	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
68	The mechanism of oxygen activation on single Pt-atom doped SnO2(110) surface. Journal of Materials Science, 2016, 51, 10400-10407.	1.7	32
69	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
70	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
71	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
72	A first principles study of O2 dissociation on Pt modified ZrC(100) surface. Chemical Physics Letters, 2016, 649, 141-147.	1.2	11

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73	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
74	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
75	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
76	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
77	First principles study of O2 adsorption on Al-doped ZnO(<unknown>) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 602 Td (unknown)ls surface. Sensors and Actuators B: Chemical, 2016, 224, 372-380.	4.0	25
78	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
79	Coadsorption of gold with chlorine on CeO ₂ (111) surfaces: A first principles study. Chinese Physics B, 2015, 24, 026801.	0.7	3
80	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
81	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
82	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
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	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
85	Graphyne as a promising substrate for the noble-metal single-atom catalysts. Carbon, 2015, 95, 756-765.	5.4	181
86	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
87	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
88	Adsorption and dissociation of ammonia on small iron clusters. International Journal of Hydrogen Energy, 2015, 40, 346-352.	3.8	23
89	CO catalytic oxidation on iron-embedded monolayer MoS2. Applied Surface Science, 2015, 328, 71-77.	3.1	100
90	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

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91	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
92	O2 activation on the outer surface of carbon nanotubes modified by encapsulated iron clusters. Applied Surface Science, 2014, 300, 91-97.	3.1	11
93	Depletion NO x Made Easy by Nitrogen Doped Graphene. Catalysis Letters, 2014, 144, 1016-1022.	1.4	16
94	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
95	A density function theory study on the NO reduction on nitrogen doped graphene. Physical Chemistry Chemical Physics, 2014, 16, 20561-20569.	1.3	53
96	Several different charge transfer and Ce³⁺localization scenarios for Rhâ€"CeO₂(111). Journal of Materials Chemistry A, 2014, 2, 2333-2345.	5.2	26
97	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
98	Sulfidation and Sulfur Recovery from SO₂ over Ceria. Journal of Physical Chemistry C, 2014, 118, 17499-17504.	1.5	11
99	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
100	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
101	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
102	Tuning the catalytic property of non-noble metallic impurities in graphene. Carbon, 2014, 71, 139-149.	5.4	85
103	The sulfur tolerance mechanism of the Cu/CeO2 system. International Journal of Hydrogen Energy, 2014, 39, 1957-1966.	3.8	5
104	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
105	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
106	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
107	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
108	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

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109	Can H2S poison the surface of yttria-stabilized zirconia?. International Journal of Hydrogen Energy, 2013, 38, 8974-8979.	3.8	16
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	Sulfidation of Ceria Surfaces from Sulfur and Sulfur Diffusion. Journal of Physical Chemistry C, 2012, 116, 8417-8425.	1.5	19
112	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
113	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
114	Cu-doped ceria: Oxygen vacancy formation made easy. Chemical Physics Letters, 2011, 510, 60-66.	1.2	53
115	SOx on ceria from adsorbed SO2. Journal of Chemical Physics, 2011, 134, 184703.	1.2	32
116	Interfacial properties of NM/CeO₂(111) (NM = noble metal atoms or clusters of Pd, Pt and) Tj ETQq0 0 0 rgBT /Overlock 10	0.7	34
117	Physisorbed, Chemisorbed, and Oxidized CO on Highly Active Cuâˆ’CeO₂(111). Journal of Physical Chemistry C, 2010, 114, 4486-4494.	1.5	110
118	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
119	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. Surface Science, 2008, 602, 1199-1206.	0.8	68
120	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
121	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
122	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
123	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
124	Oxygen vacancy formation energy in Pd-doped ceria: A DFT+U study. Journal of Chemical Physics, 2007, 127, 074704.	1.2	105
125	First-principles study of thePtâˆ•CeO2(111)interface. Physical Review B, 2007, 76, .	1.1	82
126	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

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127	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