Lei Li

List of Publications by Year
in descending order

20 papers	199 citations	1163117 8 h-index	1125743 13 g-index
20 all docs	20 docs citations	20 times ranked	181 citing authors

#	Article	IF	Citations
1	Exploring Highly Efficient Dual-Metal-Site Electrocatalysts for Oxygen Reduction Reaction by First Principles Screening. Journal of the Electrochemical Society, 2022, 169, 026524.	2.9	9
2	Computational evaluation of ScB and TiB MBenes as promising anode materials for high-performance metal-ion batteries. Physical Review Materials, 2022, 6, .	2.4	4
3	Computational screening of MBene monolayers with high electrocatalytic activity for the nitrogen reduction reaction. Nanoscale, 2021, 13, 15002-15009.	5.6	22
4	Oxygen adsorption on high-index faceted Pt nanoparticles. Physical Chemistry Chemical Physics, 2021, 23, 17323-17328.	2.8	4
5	Structural Evolution of the Surface and Interface in Bimetallic High-Index Faceted Heterogeneous Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 2454-2462.	4.6	5
6	Single Mn Atom Anchored on Nitrogenâ€Doped Graphene as a Highly Efficient Electrocatalyst for Oxygen Reduction Reaction. Chemistry - A European Journal, 2021, 27, 9686-9693.	3.3	15
7	Molecular Dynamics Simulations of Thermally Induced Surface and Shape Evolution of Concave Au Nanocubes: Implications for Catalysis. ACS Applied Nano Materials, 2021, 4, 9527-9535.	5.0	2
8	Boosting the Electrocatalytic Activity of Feâ€'Co Dualâ€Atom Catalysts for Oxygen Reduction Reaction by Ligandâ€Modification Engineering. ChemCatChem, 2021, 13, 4645-4651.	3.7	11
9	Computational screening of pristine and functionalized ordered TiVC MXenes as highly efficient anode materials for lithium-ion batteries. Nanoscale, 2021, 13, 2995-3001.	5.6	22
10	Computational screening of efficient graphene-supported transition metal single atom catalysts toward the oxygen reduction reaction. Journal of Materials Chemistry A, 2020, 8, 19319-19327.	10.3	49
11	Basin Hopping Genetic Algorithm for Global Optimization of PtCo Clusters. Journal of Chemical Information and Modeling, 2020, 60, 2219-2228.	5.4	12
12	Structural, magnetic, and electronic properties of small M-Pt (MÂ=ÂFe, Co, and Ni) clusters: Insight from density-functional calculations. Journal of Magnetism and Magnetic Materials, 2020, 512, 167047.	2.3	4
13	Thermal Stability of Unary to Quinary Noble-Metal/3d-Transition-Metal Alloy Nanoparticles from Molecular Dynamics Simulations: Implications for Multimetallic Catalysis. ACS Applied Nano Materials, 2020, 3, 5381-5389.	5.0	9
14	Structural and magnetic properties of Co-Pt clusters: A spin-polarized density functional study. Journal of Magnetism and Magnetic Materials, 2020, 503, 166651.	2.3	3
15	Solidâ€"Liquid Coexistence in Trimetallic Heterostructured Nanoparticle Catalysts: Insights from Molecular Dynamics Simulations. ACS Applied Nano Materials, 2020, 3, 12369-12378.	5.0	10
16	[2+1] Additions of (n,0)(n=6â'10) single-walled carbon nanotubes with di-vacancies based on defect curvature: A first-principles study. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950004.	1.8	1
17	Structural Transformation and Cycling Improvement of Nanosized Flower-like Î³-MnO₂ in a Sodium Battery. ACS Applied Energy Materials, 2019, 2, 5050-5056.	5.1	13
18	[1+1] and [2+1] Additions on a (5,5) Single-Walled Carbon Nanotube with V₁~V₄ Vacancies Based on Defect Curvature: A First Principles Study. Acta Chimica Sinica, 2017, 75, 284.	1.4	1

#	Article	IF	Citations
19	Curvature, vacancy size and chirality effects of mono- to octa-vacancies in zigzag single-walled carbon nanotubes. New Journal of Chemistry, 2016, 40, 8625-8631.	2.8	1
20	Molecular Dynamics Investigation on Thermal Stability and Shape Evolution of Pd-Au Heterostructured Nanorods: Implications for Catalysis. ACS Applied Nano Materials, 0, , .	5.0	2