Lei Li

List of Publications by Year
in descending order

29 papers	2,297 citations	257101 24 h-index	476904 29 g-index
29 all docs	29 docs citations	29 times ranked	3732 citing authors

#	Article	IF	Citations
1	MoS₂/MX₂ heterobilayers: bandgap engineering via tensile strain or external electrical field. Nanoscale, 2014, 6, 2879-2886.	2.8	326
2	A Theoretical Study of Single-Atom Catalysis of CO Oxidation Using Au Embedded 2D h-BN Monolayer: A CO-Promoted O2 Activation. Scientific Reports, 2014, 4, 5441.	1.6	211
3	CO Self-Promoting Oxidation on Nanosized Gold Clusters: Triangular Au₃ Active Site and CO Induced Oâ€“O Scission. Journal of the American Chemical Society, 2013, 135, 2583-2595.	6.6	178
4	Single Iridium Atom Doped Ni₂P Catalyst for Optimal Oxygen Evolution. Journal of the American Chemical Society, 2021, 143, 13605-13615.	6.6	162
5	Controlling Catalytic Properties of Pd Nanoclusters through Their Chemical Environment at the Atomic Level Using Isoreticular Metalâ€“Organic Frameworks. ACS Catalysis, 2016, 6, 3461-3468.	5.5	152
6	CO Oxidation on TiO₂ (110) Supported Subnanometer Gold Clusters: Size and Shape Effects. Journal of the American Chemical Society, 2013, 135, 19336-19346.	6.6	127
7	New Mechanistic Pathways for Criegeeâ€“Water Chemistry at the Air/Water Interface. Journal of the American Chemical Society, 2016, 138, 11164-11169.	6.6	111
8	Tuning the electronic properties of monolayer and bilayer PtSe₂via strain engineering. Journal of Materials Chemistry C, 2016, 4, 3106-3112.	2.7	96
9	Near-Barrierless Ammonium Bisulfate Formation via a Loop-Structure Promoted Proton-Transfer Mechanism on the Surface of Water. Journal of the American Chemical Society, 2016, 138, 1816-1819.	6.6	93
10	Magic-Number Gold Nanoclusters with Diameters from 1 to 3.5 nm: Relative Stability and Catalytic Activity for CO Oxidation. Nano Letters, 2015, 15, 682-688.	4.5	92
11	Characterizing hydrophobicity of amino acid side chains in a protein environment via measuring contact angle of a water nanodroplet on planar peptide network. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12946-12951.	3.3	87
12	Tuning thermal contact conductance at grapheneâ€“copper interfaceviasurface nanoengineering. Nanoscale, 2015, 7, 6286-6294.	2.8	85
13	Formation of HONO from the NH₃-promoted hydrolysis of NO₂dimers in the atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7236-7241.	3.3	67
14	PtPd(111) Surface versus PtAu(111) Surface: Which One Is More Active for Methanol Oxidation?. ACS Catalysis, 2018, 8, 132-143.	5.5	56
15	Interaction of the NH₂ Radical with the Surface of a Water Droplet. Journal of the American Chemical Society, 2015, 137, 12070-12078.	6.6	52
16	Kinetic and mechanistic investigations of the direct synthesis of dimethyl carbonate from carbon dioxide over ceria nanorod catalysts. Journal of Catalysis, 2016, 340, 295-301.	3.1	50
17	Direct Simulation Evidence of Generation of Oxygen Vacancies at the Golden Cage Au₁₆ and TiO₂ (110) Interface for CO Oxidation. Journal of the American Chemical Society, 2014, 136, 15857-15860.	6.6	48
18	Highâ€Performance Ru₁/CeO₂ Singleâ€Atom Catalyst for CO Oxidation: A Computational Exploration. ChemPhysChem, 2016, 17, 3170-3175.	1.0	47

#	Article	IF	Citations
19	Interaction of SO₂ with the Surface of a Water Nanodroplet. Journal of the American Chemical Society, 2017, 139, 17168-17174.	6.6	46
20	Simulation Evidence of Hexagonalâ€toâ€Tetragonal ZnSe Structure Transition: A Monolayer Material with a Wideâ€Range Tunable Direct Bandgap. Advanced Science, 2015, 2, 1500290.	5.6	44
21	An octane-fueled low temperature solid oxide fuel cell with Ru-free anodes. Electrochemistry Communications, 2008, 10, 1295-1298.	2.3	40
22	Revealing the Intrinsic Atomic Structure and Chemistry of Amorphous LiO₂-Containing Products in Liâ€“O₂ Batteries Using Cryogenic Electron Microscopy. Journal of the American Chemical Society, 2022, 144, 2129-2136.	6.6	28
23	High performance Niâ€“Sm2O3 cermet anodes for intermediate-temperature solid oxide fuel cells. Journal of Power Sources, 2009, 187, 400-402.	4.0	26
24	Carbon Nanotube Superarchitectures: An Ab Initio Study. Journal of Physical Chemistry C, 2011, 115, 18174-18185.	1.5	25
25	Adaptive kinetic Monte Carlo simulations of surface segregation in PdAu nanoparticles. Nanoscale, 2019, 11, 10524-10535.	2.8	25
26	Pair-distribution-function guided optimization of fingerprints for atom-centered neural network potentials. Journal of Chemical Physics, 2020, 152, 224102.	1.2	8
27	Structure transition of Au₁₈ from pyramidal to a hollow-cage during soft-landing onto a TiO₂(110) surface. Chemical Communications, 2015, 51, 9535-9538.	2.2	7
28	Resolving the HONO formation mechanism in the ionosphere via ab initio molecular dynamic simulations. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4629-4633.	3.3	4
29	Twist-to-Untwist Evolution and Cation Polarization Behavior of Hybrid Halide Perovskite Nanoplatelets Revealed by Cryogenic Transmission Electron Microscopy. Journal of Physical Chemistry Letters, 2021, 12, 12187-12195.	2.1	4