Kaining Duanmu

List of Publications by Year
in descending order

16	799	840776 11	940533 16
papers	citations	h-index	g-index

16	16	16	1459
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Concentration-Dependent Solvation Structure and Dynamics of Aqueous Sulfuric Acid Using Multinuclear NMR and DFT. Journal of Physical Chemistry B, 2021, 125, 5089-5099.	2.6	5
2	Long-Term Structural and Chemical Stability of Carbon Electrodes in Vanadium Redox Flow Battery. ACS Applied Energy Materials, 2021, 4, 6074-6081.	5.1	14
3	Mechanistic and Electronic Insights into a Working NiAu Single-Atom Alloy Ethanol Dehydrogenation Catalyst. Journal of the American Chemical Society, 2021, 143, 21567-21579.	13.7	28
4	Evolution of Metastable Structures at Bimetallic Surfaces from Microscopy and Machine-Learning Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 15907-15916.	13.7	47
5	Facilitating hydrogen atom migration via a dense phase on palladium islands to a surrounding silver surface. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 22657-22664.	7.1	26
6	Tuning reactivity layer-by-layer: formic acid activation on Ag/Pd(111). Chemical Science, 2020, 11, 6492-6499.	7.4	7
7	Automated Detection and Characterization of Surface Restructuring Events in Bimetallic Catalysts. Journal of Physical Chemistry C, 2019, 123, 16332-16344.	3.1	10
8	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. Nature Catalysis, 2019, 2, 495-503.	34.4	464
9	Validation of Density Functionals for Adsorption Energies on Transition Metal Surfaces. Journal of Chemical Theory and Computation, 2017, 13, 835-842.	5.3	40
10	Thermodynamics of Metal Nanoparticles: Energies and Enthalpies of Formation of Magnesium Clusters and Nanoparticles as Large as 1.3 nm. Journal of Physical Chemistry C, 2016, 120, 26110-26118.	3.1	18
11	Size-Dependent Ligand Quenching of Ferromagnetism in Co₃(benzene)_n ⁺ Clusters Studied with X-ray Magnetic Circular Dichroism Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 4568-4575.	4.6	27
12	Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg_n^{0,ÂÂ±Â1}, n = 1â€“7. Journal of Physical Chemistry C, 2016, 120, 13275-13286.	3.1	32
13	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. ACS Catalysis, 2015, 5, 2070-2080.	11.2	28
14	Validation of Methods for Computational Catalyst Design: Geometries, Structures, and Energies of Neutral and Charged Silver Clusters. Journal of Physical Chemistry C, 2015, 119, 9617-9626.	3.1	31
15	Atomic Oxygen Recombination at Surface Defects on Reconstructed (0001) Î±-Quartz Exposed to Atomic and Molecular Oxygen. Journal of Physical Chemistry C, 2015, 119, 9287-9301.	3.1	16
16	Partial Ionic Character beyond the Pauling Paradigm: Metal Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 28069-28074.	3.1	6