

Kaining Duanmu

List of Publications by Year in descending order

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16
papers

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840776

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times ranked

1459
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. <i>Nature Catalysis</i> , 2019, 2, 495-503. | 34.4 | 464 |
| 2 | Evolution of Metastable Structures at Bimetallic Surfaces from Microscopy and Machine-Learning Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2020, 142, 15907-15916. | 13.7 | 47 |
| 3 | Validation of Density Functionals for Adsorption Energies on Transition Metal Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 835-842. | 5.3 | 40 |
| 4 | Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: $Mg_n^0, \pm 1$, $n = 1-7$. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13275-13286. | 3.1 | 32 |
| 5 | Validation of Methods for Computational Catalyst Design: Geometries, Structures, and Energies of Neutral and Charged Silver Clusters. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9617-9626. | 3.1 | 31 |
| 6 | Density Functional Theory of the Water Splitting Reaction on Fe(O): Comparison of Local and Nonlocal Correlation Functionals. <i>ACS Catalysis</i> , 2015, 5, 2070-2080. | 11.2 | 28 |
| 7 | Mechanistic and Electronic Insights into a Working NiAu Single-Atom Alloy Ethanol Dehydrogenation Catalyst. <i>Journal of the American Chemical Society</i> , 2021, 143, 21567-21579. | 13.7 | 28 |
| 8 | Size-Dependent Ligand Quenching of Ferromagnetism in Co_3 (benzene) $_n^+$ Clusters Studied with X-ray Magnetic Circular Dichroism Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4568-4575. | 4.6 | 27 |
| 9 | Facilitating hydrogen atom migration via a dense phase on palladium islands to a surrounding silver surface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 22657-22664. | 7.1 | 26 |
| 10 | Thermodynamics of Metal Nanoparticles: Energies and Enthalpies of Formation of Magnesium Clusters and Nanoparticles as Large as 1.3 nm. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26110-26118. | 3.1 | 18 |
| 11 | Atomic Oxygen Recombination at Surface Defects on Reconstructed (0001) $\hat{\alpha}$ -Quartz Exposed to Atomic and Molecular Oxygen. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9287-9301. | 3.1 | 16 |
| 12 | Long-Term Structural and Chemical Stability of Carbon Electrodes in Vanadium Redox Flow Battery. <i>ACS Applied Energy Materials</i> , 2021, 4, 6074-6081. | 5.1 | 14 |
| 13 | Automated Detection and Characterization of Surface Restructuring Events in Bimetallic Catalysts. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16332-16344. | 3.1 | 10 |
| 14 | Tuning reactivity layer-by-layer: formic acid activation on Ag/Pd(111). <i>Chemical Science</i> , 2020, 11, 6492-6499. | 7.4 | 7 |
| 15 | Partial Ionic Character beyond the Pauling Paradigm: Metal Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28069-28074. | 3.1 | 6 |
| 16 | Concentration-Dependent Solvation Structure and Dynamics of Aqueous Sulfuric Acid Using Multinuclear NMR and DFT. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5089-5099. | 2.6 | 5 |