Guoxiang Hu

List of Publications by Year in descending order

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Version: 2024-02-01



#	Article	IF	CITATIONS
1	Insights into Interfaces, Stability, Electronic Properties, and Catalytic Activities of Atomically Precise Metal Nanoclusters from First Principles. Accounts of Chemical Research, 2018, 51, 2793-2802.	15.6	231
2	Universal Surface Engineering of Transition Metals for Superior Electrocatalytic Hydrogen Evolution in Neutral Water. Journal of the American Chemical Society, 2017, 139, 12283-12290.	13.7	207
3	Three-orders-of-magnitude variation of carrier lifetimes with crystal phase of gold nanoclusters. Science, 2019, 364, 279-282.	12.6	149
4	Machine learned features from density of states for accurate adsorption energy prediction. Nature Communications, 2021, 12, 88.	12.8	108
5	Atomically Precise Bimetallic Au ₁₉ Cu ₃₀ Nanocluster with an Icosidodecahedral Cu ₃₀ Shell and an Alkynyl–Cu Interface. Journal of the American Chemical Society, 2017, 139, 9451-9454.	13.7	104
6	Ta–TiOx nanoparticles as radical scavengers to improve the durability of Fe–N–C oxygen reduction catalysts. Nature Energy, 2022, 7, 281-289.	39.5	93
7	Diphosphine-Protected Au ₂₂ Nanoclusters on Oxide Supports Are Active for Gas-Phase Catalysis without Ligand Removal. Nano Letters, 2016, 16, 6560-6567.	9.1	88
8	CoP for hydrogen evolution: implications from hydrogen adsorption. Physical Chemistry Chemical Physics, 2016, 18, 23864-23871.	2.8	84
9	Effects of Metal-Doping on Hydrogen Evolution Reaction Catalyzed by MAu ₂₄ and M ₂ Au ₃₆ Nanoclusters (M = Pt, Pd). ACS Applied Materials & Interfaces, 2018, 10, 44645-44653.	8.0	81
10	Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-Doped Graphene. Journal of Physical Chemistry C, 2020, 124, 19571-19578.	3.1	75
11	Metallic Hydrogen in Atomically Precise Gold Nanoclusters. Chemistry of Materials, 2017, 29, 4840-4847.	6.7	70
12	Stronger-than-Pt hydrogen adsorption in a Au ₂₂ nanocluster for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2018, 6, 7532-7537.	10.3	63
13	Selective CO Production by Photoelectrochemical Methane Oxidation on TiO ₂ . ACS Central Science, 2018, 4, 631-637.	11.3	56
14	Thiolate-Protected Trimetallic Au _{â^¼20} Ag _{â^¼4} Pd and Au _{â^¼20} Ag _{â^¼4} Pt Alloy Clusters with Controlled Chemical Composition and Metal Positions. Journal of Physical Chemistry Letters, 2018, 9, 2590-2594.	4.6	55
15	Interface Engineering of Earth-Abundant Transition Metals Using Boron Nitride for Selective Electroreduction of CO ₂ . ACS Applied Materials & Interfaces, 2018, 10, 6694-6700.	8.0	52
16	First Principles Insight into H ₂ Activation and Hydride Species on TiO ₂ Surfaces. Journal of Physical Chemistry C, 2018, 122, 20323-20328.	3.1	44
17	Beyond the staple motif: a new order at the thiolate–gold interface. Nanoscale, 2016, 8, 20103-20110.	5.6	32
18	Kinetics and Mechanism of Methanol Conversion over Anatase Titania Nanoshapes. ACS Catalysis, 2017, 7, 5345-5356.	11.2	31

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19	Superior electrocatalytic hydrogen evolution at engineered non-stoichiometric two-dimensional transition metal dichalcogenide edges. Journal of Materials Chemistry A, 2019, 7, 18357-18364.	10.3	30
20	Electronic band contraction induced low temperature methane activation on metal alloys. Journal of Materials Chemistry A, 2020, 8, 6057-6066.	10.3	28
21	Predicting synthesizable multi-functional edge reconstructions in two-dimensional transition metal dichalcogenides. Npj Computational Materials, 2020, 6, .	8.7	23
22	Fluorescence of Hydroxyphenyl-Substituted "Click―Triazoles. Journal of Physical Chemistry A, 2018, 122, 2956-2973.	2.5	21
23	Methane Chemisorption on Oxideâ€Supported Pt Single Atom. ChemPhysChem, 2019, 20, 2217-2220.	2.1	19
24	Hydrogen in Nanocatalysis. Journal of Physical Chemistry Letters, 2020, 11, 7049-7057.	4.6	18
25	Work Function Engineering of 2D Materials: The Role of Polar Edge Reconstructions. Journal of Physical Chemistry Letters, 2021, 12, 2320-2326.	4.6	18
26	A combined first principles study of the structural, magnetic, and phonon properties of monolayer CrI3. Journal of Chemical Physics, 2022, 156, 014707.	3.0	18
27	Inverse design of two-dimensional materials with invertible neural networks. Npj Computational Materials, 2021, 7, .	8.7	15
28	Fundamental Flaw in the Current Construction of the TiO ₂ Electron Transport Layer of Perovskite Solar Cells and Its Elimination. ACS Applied Materials & Interfaces, 2021, 13, 39371-39378.	8.0	11
29	Reversible Hydrogen-Induced Phase Transformations in La _{0.7} Sr _{0.3} MnO ₃ Thin Films Characterized by In Situ Neutron Reflectometry. ACS Applied Materials & Interfaces, 2022, 14, 10898-10906.	8.0	10
30	Voltage-Driven Molecular Catalysis of Electrochemical Reactions. Journal of the American Chemical Society, 2021, 143, 17344-17347.	13.7	8
31	Strong Bidentate Coordination for Surface Passivation and Ligand-Shell Engineering of Lead Halide Perovskite Nanocrystals in the Strongly Quantum-Confined Regime. Journal of Physical Chemistry C, 2021, 125, 24521-24530.	3.1	4
32	Shifting and Breaking Scaling Relations at Transition Metal Telluride Edges for Selective Electrochemical CO ₂ Reduction. Journal of Materials Chemistry A, 0, , .	10.3	4
33	Dual Roles of Polymeric Capping Ligands in the Surface-Protected Etching of Colloidal Silica. ACS Applied Materials & Interfaces, 2020, 12, 38751-38756.	8.0	2