Zhenhua Zeng

List of Publications by Year
in descending order

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45 papers	5,067 citations	279798 23 h-index	254184 43 g-index
45 all docs	45 docs citations	45 times ranked	8165 citing authors

#	Article	IF	Citations
1	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
2	Exceptional Size-Dependent Activity Enhancement in the Electroreduction of CO₂ over Au Nanoparticles. Journal of the American Chemical Society, 2014, 136, 16473-16476.	13.7	600
3	In-situ structure and catalytic mechanism of NiFe and CoFe layered double hydroxides during oxygen evolution. Nature Communications, 2020, 11, 2522.	12.8	594
4	Tunable intrinsic strain in two-dimensional transition metal electrocatalysts. Science, 2019, 363, 870-874.	12.6	384
5	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3dâ€Transition Metal Layered Double Hydroxides. Angewandte Chemie - International Edition, 2021, 60, 14446-14457.	13.8	170
6	Stabilization of ultrathin (hydroxy)oxide films on transition metal substrates for electrochemical energy conversion. Nature Energy, 2017, 2, .	39.5	167
7	In Situ Oxidation Study of Pt(110) and Its Interaction with CO. Journal of the American Chemical Society, 2011, 133, 20319-20325.	13.7	120
8	Platinum-nickel hydroxide nanocomposites for electrocatalytic reduction of water. Nano Energy, 2017, 31, 456-461.	16.0	119
9	Towards First Principles-Based Prediction of Highly Accurate Electrochemical Pourbaix Diagrams. Journal of Physical Chemistry C, 2015, 119, 18177-18187.	3.1	97
10	Generalized trends in the formation energies of perovskite oxides. Physical Chemistry Chemical Physics, 2013, 15, 7526.	2.8	85
11	Coreâ€“Shell Nanostructured Cobaltâ€“Platinum Electrocatalysts with Enhanced Durability. ACS Catalysis, 2018, 8, 35-42.	11.2	72
12	Theory of nitride oxide adsorption on transition metal (111) surfaces: a first-principles investigation. Physical Chemistry Chemical Physics, 2010, 12, 2459.	2.8	63
13	Direct methane activation by atomically thin platinum nanolayers on two-dimensional metal carbides. Nature Catalysis, 2021, 4, 882-891.	34.4	63
14	Plating Precious Metals on Nonprecious Metal Nanoparticles for Sustainable Electrocatalysts. Nano Letters, 2017, 17, 3391-3395.	9.1	61
15	Avoiding pitfalls in the modeling of electrochemical interfaces. Chemical Physics Letters, 2013, 555, 145-148.	2.6	50
16	Characterization of oxygenated species at water/Pt(111) interfaces from DFT energetics and XPS simulations. Nano Energy, 2016, 29, 369-377.	16.0	47
17	Density functional theory study of the energetics, electronic structure, and core-level shifts of NO adsorption on the Pt(111) surface. Physical Review B, 2009, 79, .	3.2	45
18	Establishing and Understanding Adsorptionâ€“Energy Scaling Relations with Negative Slopes. Journal of Physical Chemistry Letters, 2016, 7, 5302-5306.	4.6	43

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19	Adsorption of NO on the Rh₁₃, Pd₁₃, Ir₁₃, and Pt₁₃ Clusters: A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2012, 116, 20540-20549.	3.1	33
20	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3dâ€Transition Metal Layered Double Hydroxides. Angewandte Chemie, 2021, 133, 14567-14578.	2.0	30
21	First-Principles Study of Carbon Monoxide Oxidation on Ag(111) in Presence of Subsurface Oxygen and Stepped Ag(221). Journal of Physical Chemistry C, 2009, 113, 8266-8272.	3.1	27
22	Influence of controlled surface oxidation on the magnetic anisotropy of Co ultrathin films. Applied Physics Letters, 2015, 106, .	3.3	27
23	First-principles calculation of core-level binding energy shift in surface chemical processes. Science China Chemistry, 2010, 53, 402-410.	8.2	25
24	Electrochemical Surface Stress Development during CO and NO Oxidation on Pt. Journal of Physical Chemistry C, 2016, 120, 8674-8683.	3.1	22
25	Theoretical study of CO adsorption on Au catalysts under environmental catalytic conditions. Catalysis Communications, 2014, 52, 78-83.	3.3	20
26	DFT Insights into NO Electrochemical Reduction: A Case Study of Pt(211) and Cu(211) Surfaces. ACS Catalysis, 2022, 12, 1394-1402.	11.2	19
27	Density functional theory andab initiomolecular dynamics study of NO adsorption on Pd(111) and Pt(111) surfaces. Physical Review B, 2010, 81, .	3.2	16
28	Origin of electrolyte-dopant dependent sulfur poisoning of SOFC anodes. Physical Chemistry Chemical Physics, 2013, 15, 6769.	2.8	15
29	In situ surface stress measurement and computational analysis examining the oxygen reduction reaction on Pt and Pd. Electrochimica Acta, 2018, 260, 400-406.	5.2	14
30	Magnetic field-induced capacitance change in aqueous carbon-based supercapacitors. Cell Reports Physical Science, 2021, 2, 100455.	5.6	13
31	Ab Initio Thermodynamic Modeling of Electrified Metalâ€“Oxide Interfaces: Consistent Treatment of Electronic and Ionic Chemical Potentials. Journal of Physical Chemistry C, 2014, 118, 22663-22671.	3.1	11
32	K-Edge XANES Investigation of Fe-Based Oxides by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2021, 125, 26229-26239.	3.1	11
33	First-principles investigation of electrochemical dissolution of Pt nanoparticles and kinetic simulation. Journal of Chemical Physics, 2019, 151, 234711.	3.0	10
34	Structural and Chemical Transformations of Zinc Oxide Ultrathin Films on Pd(111) Surfaces. ACS Applied Materials & Interfaces, 2021, 13, 35113-35123.	8.0	10
35	Mitigation of RuO₆ octahedron distortion by enhanced A-site electronegativity in pyrochlore for acidic water oxidation. Journal of Materials Chemistry A, 2022, 10, 9419-9426.	10.3	10
36	Dynamic Surface Stress Response during Reversible Mg Electrodeposition and Stripping. Journal of the Electrochemical Society, 2016, 163, A2679-A2684.	2.9	9

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37	Migration of Cobalt Species within Mixed Platinum-Cobalt Oxide Bifunctional Electrocatalysts in Alkaline Electrolytes. Journal of the Electrochemical Society, 2019, 166, F3093-F3097.	2.9	7
38	On the relationship between potential of zero charge and solvent dynamics in the reversible hydrogen electrode. Journal of Catalysis, 2021, 398, 161-170.	6.2	7
39	Direct Demonstration of Unified BrÃ¸nstedâ€'Evansâ€'Polanyi Relationships for Proton-Coupled Electron Transfer Reactions on Transition Metal Surfaces. Journal of the Electrochemical Society, 2020, 167, 166516.	2.9	7
40	Strain and support effects on phase transition and surface reactivity of ultrathin ZnO films: DFT insights. AIP Advances, 2020, 10, .	1.3	4
41	Effect of cobalt addition on platinum supported on multi-walled carbon nanotubes for water-gas shift. Journal of Catalysis, 2020, 391, 25-34.	6.2	3
42	Achieving flexible large-scale reactivity tuning by controlling the phase, thickness and support of two-dimensional ZnO. Chemical Science, 2021, 12, 15284-15290.	7.4	3
43	Band structure and Fermi surface of atomically uniform lead films. New Journal of Physics, 2010, 12, 113034.	2.9	1
44	Toward a Fundamental Understanding of Strain Generation and Strain Tuning for the Fuel Cell Applications. ECS Meeting Abstracts, 2022, MA2022-01, 1488-1488.	0.0	0
45	Catalytically-Active Phases and Reaction Mechanism of Ni-Based and Co-Based Layered Double Hydroxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2022, MA2022-01, 1368-1368.	0.0	0