

Zhenhua Zeng

List of Publications by Year in descending order

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45
papers

5,067
citations

279487

23
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253896

43
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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. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 273002.	0.7	1,933
2	Exceptional Size-Dependent Activity Enhancement in the Electroreduction of CO ₂ over Au Nanoparticles. <i>Journal of the American Chemical Society</i> , 2014, 136, 16473-16476.	6.6	600
3	In-situ structure and catalytic mechanism of NiFe and CoFe layered double hydroxides during oxygen evolution. <i>Nature Communications</i> , 2020, 11, 2522.	5.8	594
4	Tunable intrinsic strain in two-dimensional transition metal electrocatalysts. <i>Science</i> , 2019, 363, 870-874.	6.0	384
5	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3dâ€”Transition Metal Layered Double Hydroxides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 14446-14457.	7.2	170
6	Stabilization of ultrathin (hydroxy)oxide films on transition metal substrates for electrochemical energy conversion. <i>Nature Energy</i> , 2017, 2, .	19.8	167
7	In Situ Oxidation Study of Pt(110) and Its Interaction with CO. <i>Journal of the American Chemical Society</i> , 2011, 133, 20319-20325.	6.6	120
8	Platinum-nickel hydroxide nanocomposites for electrocatalytic reduction of water. <i>Nano Energy</i> , 2017, 31, 456-461.	8.2	119
9	Towards First Principles-Based Prediction of Highly Accurate Electrochemical Pourbaix Diagrams. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18177-18187.	1.5	97
10	Generalized trends in the formation energies of perovskite oxides. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7526.	1.3	85
11	Coreâ€”Shell Nanostructured Cobaltâ€”Platinum Electrocatalysts with Enhanced Durability. <i>ACS Catalysis</i> , 2018, 8, 35-42.	5.5	72
12	Theory of nitride oxide adsorption on transition metal (111) surfaces: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2459.	1.3	63
13	Direct methane activation by atomically thin platinum nanolayers on two-dimensional metal carbides. <i>Nature Catalysis</i> , 2021, 4, 882-891.	16.1	63
14	Plating Precious Metals on Nonprecious Metal Nanoparticles for Sustainable Electrocatalysts. <i>Nano Letters</i> , 2017, 17, 3391-3395.	4.5	61
15	Avoiding pitfalls in the modeling of electrochemical interfaces. <i>Chemical Physics Letters</i> , 2013, 555, 145-148.	1.2	50
16	Characterization of oxygenated species at water/Pt(111) interfaces from DFT energetics and XPS simulations. <i>Nano Energy</i> , 2016, 29, 369-377.	8.2	47
17	Density functional theory study of the energetics, electronic structure, and core-level shifts of NO adsorption on the Pt(111) surface. <i>Physical Review B</i> , 2009, 79, .	1.1	45
18	Establishing and Understanding Adsorptionâ€”Energy Scaling Relations with Negative Slopes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5302-5306.	2.1	43

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19	Adsorption of NO on the Rh ₁₃ , Pd ₁₃ , Ir ₁₃ , and Pt ₁₃ Clusters: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20540-20549.	1.5	33
20	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3d-Transition Metal Layered Double Hydroxides. <i>Angewandte Chemie</i> , 2021, 133, 14567-14578.	1.6	30
21	First-Principles Study of Carbon Monoxide Oxidation on Ag(111) in Presence of Subsurface Oxygen and Stepped Ag(221). <i>Journal of Physical Chemistry C</i> , 2009, 113, 8266-8272.	1.5	27
22	Influence of controlled surface oxidation on the magnetic anisotropy of Co ultrathin films. <i>Applied Physics Letters</i> , 2015, 106, .	1.5	27
23	First-principles calculation of core-level binding energy shift in surface chemical processes. <i>Science China Chemistry</i> , 2010, 53, 402-410.	4.2	25
24	Electrochemical Surface Stress Development during CO and NO Oxidation on Pt. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8674-8683.	1.5	22
25	Theoretical study of CO adsorption on Au catalysts under environmental catalytic conditions. <i>Catalysis Communications</i> , 2014, 52, 78-83.	1.6	20
26	DFT Insights into NO Electrochemical Reduction: A Case Study of Pt(211) and Cu(211) Surfaces. <i>ACS Catalysis</i> , 2022, 12, 1394-1402.	5.5	19
27	Density functional theory and <i>ab initio</i> molecular dynamics study of NO adsorption on Pd(111) and Pt(111) surfaces. <i>Physical Review B</i> , 2010, 81, .	1.1	16
28	Origin of electrolyte-dopant dependent sulfur poisoning of SOFC anodes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6769.	1.3	15
29	In situ surface stress measurement and computational analysis examining the oxygen reduction reaction on Pt and Pd. <i>Electrochimica Acta</i> , 2018, 260, 400-406.	2.6	14
30	Magnetic field-induced capacitance change in aqueous carbon-based supercapacitors. <i>Cell Reports Physical Science</i> , 2021, 2, 100455.	2.8	13
31	Ab Initio Thermodynamic Modeling of Electrified Metal-Oxide Interfaces: Consistent Treatment of Electronic and Ionic Chemical Potentials. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22663-22671.	1.5	11
32	K-Edge XANES Investigation of Fe-Based Oxides by Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 26229-26239.	1.5	11
33	First-principles investigation of electrochemical dissolution of Pt nanoparticles and kinetic simulation. <i>Journal of Chemical Physics</i> , 2019, 151, 234711.	1.2	10
34	Structural and Chemical Transformations of Zinc Oxide Ultrathin Films on Pd(111) Surfaces. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 35113-35123.	4.0	10
35	Mitigation of RuO ₆ octahedron distortion by enhanced A-site electronegativity in pyrochlore for acidic water oxidation. <i>Journal of Materials Chemistry A</i> , 2022, 10, 9419-9426.	5.2	10
36	Dynamic Surface Stress Response during Reversible Mg Electrodeposition and Stripping. <i>Journal of the Electrochemical Society</i> , 2016, 163, A2679-A2684.	1.3	9

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37	Migration of Cobalt Species within Mixed Platinum-Cobalt Oxide Bifunctional Electrocatalysts in Alkaline Electrolytes. <i>Journal of the Electrochemical Society</i> , 2019, 166, F3093-F3097.	1.3	7
38	On the relationship between potential of zero charge and solvent dynamics in the reversible hydrogen electrode. <i>Journal of Catalysis</i> , 2021, 398, 161-170.	3.1	7
39	Direct Demonstration of Unified Brønsted-Evans-Polanyi Relationships for Proton-Coupled Electron Transfer Reactions on Transition Metal Surfaces. <i>Journal of the Electrochemical Society</i> , 2020, 167, 166516.	1.3	7
40	Strain and support effects on phase transition and surface reactivity of ultrathin ZnO films: DFT insights. <i>AIP Advances</i> , 2020, 10, .	0.6	4
41	Effect of cobalt addition on platinum supported on multi-walled carbon nanotubes for water-gas shift. <i>Journal of Catalysis</i> , 2020, 391, 25-34.	3.1	3
42	Achieving flexible large-scale reactivity tuning by controlling the phase, thickness and support of two-dimensional ZnO. <i>Chemical Science</i> , 2021, 12, 15284-15290.	3.7	3
43	Band structure and Fermi surface of atomically uniform lead films. <i>New Journal of Physics</i> , 2010, 12, 113034.	1.2	1
44	Toward a Fundamental Understanding of Strain Generation and Strain Tuning for the Fuel Cell Applications. <i>ECS Meeting Abstracts</i> , 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. <i>ECS Meeting Abstracts</i> , 2022, MA2022-01, 1368-1368.	0.0	0