Tao Cheng

List of Publications by Year
in descending order

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115 papers	9,528 citations	57631 44 h-index	39575 94 g-index
117 all docs	117 docs citations	117 times ranked	9223 citing authors

#	Article	IF	Citations
1	Ultrafine jagged platinum nanowires enable ultrahigh mass activity for the oxygen reduction reaction. Science, 2016, 354, 1414-1419.	6.0	1,292
2	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. Nature Catalysis, 2019, 2, 495-503.	16.1	464
3	Full atomistic reaction mechanism with kinetics for CO reduction on Cu(100) from ab initio molecular dynamics free-energy calculations at 298 K. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1795-1800.	3.3	414
4	Mechanistic Explanation of the pH Dependence and Onset Potentials for Hydrocarbon Products from Electrochemical Reduction of CO on Cu (111). Journal of the American Chemical Society, 2016, 138, 483-486.	6.6	381
5	Subsurface oxide plays a critical role in CO ₂ activation by Cu(111) surfaces to form chemisorbed CO ₂ , the first step in reduction of CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6706-6711.	3.3	363
6	Cu metal embedded in oxidized matrix catalyst to promote CO ₂ activation and CO dimerization for electrochemical reduction of CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6685-6688.	3.3	322
7	Atomistic Mechanisms Underlying Selectivities in C₁ and C₂ Products from Electrochemical Reduction of CO on Cu(111). Journal of the American Chemical Society, 2017, 139, 130-136.	6.6	320
8	Reaction Mechanisms for the Electrochemical Reduction of CO₂ to CO and Formate on the Cu(100) Surface at 298 K from Quantum Mechanics Free Energy Calculations with Explicit Water. Journal of the American Chemical Society, 2016, 138, 13802-13805.	6.6	310
9	Highly active and stable stepped Cu surface for enhanced electrochemical CO2 reduction to C2H4. Nature Catalysis, 2020, 3, 804-812.	16.1	298
10	Explanation of Dramatic pH-Dependence of Hydrogen Binding on Noble Metal Electrode: Greatly Weakened Water Adsorption at High pH. Journal of the American Chemical Society, 2018, 140, 7787-7790.	6.6	234
11	Formation of carbonâ€“nitrogen bonds in carbon monoxide electrolysis. Nature Chemistry, 2019, 11, 846-851.	6.6	223
12	Free-Energy Barriers and Reaction Mechanisms for the Electrochemical Reduction of CO on the Cu(100) Surface, Including Multiple Layers of Explicit Solvent at pH 0. Journal of Physical Chemistry Letters, 2015, 6, 4767-4773.	2.1	206
13	Ultrahigh Mass Activity for Carbon Dioxide Reduction Enabled by Goldâ€“Iron Coreâ€“Shell Nanoparticles. Journal of the American Chemical Society, 2017, 139, 15608-15611.	6.6	191
14	Te-Doped Pd Nanocrystal for Electrochemical Urea Production by Efficiently Coupling Carbon Dioxide Reduction with Nitrite Reduction. Nano Letters, 2020, 20, 8282-8289.	4.5	188
15	Alloying Nickel with Molybdenum Significantly Accelerates Alkaline Hydrogen Electrocatalysis. Angewandte Chemie - International Edition, 2021, 60, 5771-5777.	7.2	182
16	Weakening hydrogen adsorption on nickel via interstitial nitrogen doping promotes bifunctional hydrogen electrocatalysis in alkaline solution. Energy and Environmental Science, 2019, 12, 3522-3529.	15.6	177
17	Electrochemical CO Reduction Builds Solvent Water into Oxygenate Products. Journal of the American Chemical Society, 2018, 140, 9337-9340.	6.6	170
18	Boosting electrocatalytic CO2â€“toâ€“ethanol production via asymmetric Câ€“C coupling. Nature Communications, 2022, 13, .	5.8	158

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19	Nature of the Active Sites for CO Reduction on Copper Nanoparticles; Suggestions for Optimizing Performance. Journal of the American Chemical Society, 2017, 139, 11642-11645.	6.6	146
20	Atomistic Explanation of Shear-Induced Amorphous Band Formation in Boron Carbide. Physical Review Letters, 2014, 113, 095501.	2.9	138
21	A Highly Active Star Decahedron Cu Nanocatalyst for Hydrocarbon Production at Low Overpotentials. Advanced Materials, 2019, 31, e1805405.	11.1	134
22	Electrocatalysis at Organicâ€“Metal Interfaces: Identification of Structureâ€“Reactivity Relationships for CO₂ Reduction at Modified Cu Surfaces. Journal of the American Chemical Society, 2019, 141, 7355-7364.	6.6	133
23	Single-site Pt-doped RuO ₂ hollow nanospheres with interstitial C for high-performance acidic overall water splitting. Science Advances, 2022, 8, eabl9271.	4.7	117
24	Identifying Active Sites for CO₂ Reduction on Dealloyed Gold Surfaces by Combining Machine Learning with Multiscale Simulations. Journal of the American Chemical Society, 2019, 141, 11651-11657.	6.6	107
25	Selective CO₂ Electrochemical Reduction Enabled by a Tricomponent Copolymer Modifier on a Copper Surface. Journal of the American Chemical Society, 2021, 143, 2857-2865.	6.6	104
26	Initial Steps of Thermal Decomposition of Dihydroxylammonium 5,5â€²-bistetrazole-1,1â€²-diolate Crystals from Quantum Mechanics. Journal of Physical Chemistry C, 2014, 118, 27175-27181.	1.5	101
27	Discrete Dimers of Redox-Active and Fluorescent Perylene Diimide-Based Rigid Isosceles Triangles in the Solid State. Journal of the American Chemical Society, 2019, 141, 1290-1303.	6.6	87
28	Identification of the Selective Sites for Electrochemical Reduction of CO to C₂₊ Products on Copper Nanoparticles by Combining Reactive Force Fields, Density Functional Theory, and Machine Learning. ACS Energy Letters, 2018, 3, 2983-2988.	8.8	73
29	Rational Molecular Design of Dibenzo[a,c]phenazine-Based Thermally Activated Delayed Fluorescence Emitters for Orange-Red OLEDs with EQE up to 22.0%. ACS Applied Materials & Interfaces, 2019, 11, 26144-26151.	4.0	73
30	Reaction intermediates during operando electrocatalysis identified from full solvent quantum mechanics molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7718-7722.	3.3	70
31	tert-Butyl substituted hetero-donor TADF compounds for efficient solution-processed non-doped blue OLEDs. Journal of Materials Chemistry C, 2020, 8, 5769-5776.	2.7	68
32	Anisotropic Impact Sensitivity and Shock Induced Plasticity of TKX-50 (Dihydroxylammonium) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 Journal of Physical Chemistry C, 2015, 119, 2196-2207.	1.5	67
33	Synergized Cu/Pb Core/Shell Electrocatalyst for High-Efficiency CO₂ Reduction to C₂₊ Liquids. ACS Nano, 2021, 15, 1039-1047.	7.3	64
34	Au-activated N motifs in non-coherent cupric porphyrin metal organic frameworks for promoting and stabilizing ethylene production. Nature Communications, 2022, 13, 63.	5.8	64
35	Dramatic differences in carbon dioxide adsorption and initial steps of reduction between silver and copper. Nature Communications, 2019, 10, 1875.	5.8	63
36	Fastening Br^{â€“} Ions at Copperâ€“Molecule Interface Enables Highly Efficient Electroreduction of CO₂ to Ethanol. ACS Energy Letters, 2021, 6, 437-444.	8.8	62

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37	Molecular Russian dolls. Nature Communications, 2018, 9, 5275.	5.8	61
38	Surface Ligand Promotion of Carbon Dioxide Reduction through Stabilizing Chemisorbed Reactive Intermediates. Journal of Physical Chemistry Letters, 2018, 9, 3057-3061.	2.1	61
39	Highâ€Performance Nondoped Blue Delayed Fluorescence Organic Lightâ€Emitting Diodes Featuring Low Driving Voltage and High Brightness. Advanced Science, 2020, 7, 1902508.	5.6	60
40	Pb-Activated Amine-Assisted Photocatalytic Hydrogen Evolution Reaction on Organicâ€“Inorganic Perovskites. Journal of the American Chemical Society, 2018, 140, 1994-1997.	6.6	59
41	Bismuth Oxyhydroxide-Pt Inverse Interface for Enhanced Methanol Electrooxidation Performance. Nano Letters, 2020, 20, 7751-7759.	4.5	58
42	Atomistic Explanation of the Dramatically Improved Oxygen Reduction Reaction of Jagged Platinum Nanowires, 50 Times Better than Pt. Journal of the American Chemical Society, 2020, 142, 8625-8632.	6.6	55
43	Adaptive Accelerated ReaxFF Reactive Dynamics with Validation from Simulating Hydrogen Combustion. Journal of the American Chemical Society, 2014, 136, 9434-9442.	6.6	53
44	Compressed Intermetallic PdCu for Enhanced Electrocatalysis. ACS Energy Letters, 2020, 5, 3672-3680.	8.8	50
45	Benzo-Fused Periacenes or Double Helicenes? Different Cyclodehydrogenation Pathways on Surface and in Solution. Journal of the American Chemical Society, 2019, 141, 7399-7406.	6.6	49
46	Bimetallic PdAu Nanoframes for Electrochemical H₂O₂ Production in Acids. , 2021, 3, 996-1002.		48
47	Promoting Mechanistic Understanding of Lithium Deposition and Solidâ€Electrolyte Interphase (SEI) Formation Using Advanced Characterization and Simulation Methods: Recent Progress, Limitations, and Future Perspectives. Advanced Energy Materials, 2022, 12, .	10.2	47
48	Controllable CO adsorption determines ethylene and methane productions from CO2 electroreduction. Science Bulletin, 2021, 66, 62-68.	4.3	45
49	Efficient Orangeâ€“Red Delayed Fluorescence Organic Lightâ€Emitting Diodes with External Quantum Efficiency over 26%. Advanced Electronic Materials, 2020, 6, 1900843.	2.6	44
50	Mechanism and kinetics of the electrocatalytic reaction responsible for the high cost of hydrogen fuel cells. Physical Chemistry Chemical Physics, 2017, 19, 2666-2673.	1.3	43
51	Predicted Structures of the Active Sites Responsible for the Improved Reduction of Carbon Dioxide by Gold Nanoparticles. Journal of Physical Chemistry Letters, 2017, 8, 3317-3320.	2.1	43
52	The DFT-ReaxFF Hybrid Reactive Dynamics Method with Application to the Reductive Decomposition Reaction of the TFSI and DOL Electrolyte at a Lithiumâ€“Metal Anode Surface. Journal of Physical Chemistry Letters, 2021, 12, 1300-1306.	2.1	43
53	Anomalous Size Effect of Pt Ultrathin Nanowires on Oxygen Reduction Reaction. Nano Letters, 2021, 21, 9354-9360.	4.5	43
54	Annealing kinetics of electrodeposited lithium dendrites. Journal of Chemical Physics, 2015, 143, 134701.	1.2	42

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55	Intramolecular Energy and Electron Transfer within a Diazaperopyrenium-Based Cyclophane. Journal of the American Chemical Society, 2017, 139, 4107-4116.	6.6	42
56	Enhanced electroreduction of CO2 to C2+ products on heterostructured Cu/oxide electrodes. CheM, 2022, 8, 2148-2162.	5.8	41
57	Size-Matched Radical Multivalency. Journal of the American Chemical Society, 2017, 139, 3986-3998.	6.6	39
58	Rescaling of metal oxide nanocrystals for energy storage having high capacitance and energy density with robust cycle life. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7914-7919.	3.3	38
59	Initial decomposition reaction of di-tetrazine-tetroxide (DTTO) from quantum molecular dynamics: implications for a promising energetic material. Journal of Materials Chemistry A, 2015, 3, 1972-1978.	5.2	38
60	Highly Selective Electrocatalytic Reduction of CO₂ into Methane on Cuâ€“Bi Nanoalloys. Journal of Physical Chemistry Letters, 2020, 11, 7261-7266.	2.1	37
61	Alloying Nickel with Molybdenum Significantly Accelerates Alkaline Hydrogen Electrocatalysis. Angewandte Chemie, 2021, 133, 5835-5841.	1.6	37
62	Autobifunctional Mechanism of Jagged Pt Nanowires for Hydrogen Evolution Kinetics via End-to-End Simulation. Journal of the American Chemical Society, 2021, 143, 5355-5363.	6.6	33
63	Effects of High and Low Salt Concentrations in Electrolytes at Lithiumâ€“Metal Anode Surfaces Using DFT-ReaxFF Hybrid Molecular Dynamics Method. Journal of Physical Chemistry Letters, 2021, 12, 2922-2929.	2.1	32
64	On the accuracy of predicting shear viscosity of molecular liquids using the periodic perturbation method. Journal of Chemical Physics, 2008, 129, 144501.	1.2	31
65	Boosting hydrogen production with ultralow working voltage by selenium vacancyâ€enhanced ultrafine platinumâ€“nickel nanowires. SmartMat, 2022, 3, 130-141.	6.4	30
66	Influence of Constitution and Charge on Radical Pairing Interactions in Tris-radical Tricationic Complexes. Journal of the American Chemical Society, 2016, 138, 8288-8300.	6.6	29
67	First-principlesâ€“based reaction kinetics from reactive molecular dynamics simulations: Application to hydrogen peroxide decomposition. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18202-18208.	3.3	29
68	Approaching 100% Selectivity at Low Potential on Ag for Electrochemical CO₂ Reduction to CO Using a Surface Additive. ACS Catalysis, 2021, 11, 9034-9042.	5.5	29
69	Surface engineering of RhOOH nanosheets promotes hydrogen evolution in alkaline. Nano Energy, 2020, 78, 105224.	8.2	27
70	Molecular engineering of microporous crystals: (IV) Crystallization process of microporous aluminophosphate AlPO4-11. Microporous and Mesoporous Materials, 2012, 152, 190-207.	2.2	26
71	Sulfur-doped graphene anchoring of ultrafine Au25 nanoclusters for electrocatalysis. Nano Research, 2021, 14, 3509-3513.	5.8	26
72	Coreâ€“shell nanoparticles with tensile strain enable highly efficient electrochemical ethanol oxidation. Journal of Materials Chemistry A, 2021, 9, 15373-15380.	5.2	26

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73	Rh/RhO_x nanosheets as pH-universal bifunctional catalysts for hydrazine oxidation and hydrogen evolution reactions. Journal of Materials Chemistry A, 2022, 10, 1891-1898.	5.2	25
74	N-modulated Cu+ for efficient electrochemical carbon monoxide reduction to acetate. Science China Materials, 2020, 63, 2606-2612.	3.5	24
75	Predicted Operando Polymerization at Lithium Anode via Boron Insertion. ACS Energy Letters, 2021, 6, 2320-2327.	8.8	24
76	Neighboring Component Effect in a Tri-stable [2]Rotaxane. Journal of the American Chemical Society, 2018, 140, 13827-13834.	6.6	22
77	Pathway of in situ polymerization of 1,3-dioxolane in LiPF6 electrolyte on Li metal anode. Materials Today Energy, 2021, 21, 100730.	2.5	22
78	Predicted detonation properties at the Chapmanâ€“Jouguet state for proposed energetic materials (MTO) Tj ETQq0 0 0 rgBT /Overlock 1 Chemical Physics, 2018, 20, 3953-3969.	1.3	21
79	One force field for predicting multiple thermodynamic properties of liquid and vapor ethylene oxide. Fluid Phase Equilibria, 2008, 274, 36-43.	1.4	20
80	Synergy between a Silverâ€“Copper Surface Alloy Composition and Carbon Dioxide Adsorption and Activation. ACS Applied Materials & Interfaces, 2020, 12, 25374-25382.	4.0	19
81	Classic Force Field for Predicting Surface Tension and Interfacial Properties of Sodium Dodecyl Sulfate. Journal of Physical Chemistry B, 2010, 114, 13736-13744.	1.2	18
82	Adsorption of Ethanol Vapor on Mica Surface under Different Relative Humidities: A Molecular Simulation Study. Journal of Physical Chemistry C, 2012, 116, 16436-16446.	1.5	18
83	Reaction mechanism from quantum molecular dynamics for the initial thermal decomposition of 2,4,6-triamino-1,3,5-triazine-1,3,5-trioxide (MTO) and 2,4,6-trinitro-1,3,5-triazine-1,3,5-trioxide (MTO3N), promising green energetic materials. Journal of Materials Chemistry A, 2015, 3, 12044-12050.	5.2	18
84	Initial Decomposition Reactions of Bicyclo-HMX [BCHMX or cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole] from Quantum Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 2290-2296.	1.5	17
85	Epitaxial growth of cobalt oxide phases on Ru(0001) for spintronic device applications. Semiconductor Science and Technology, 2017, 32, 095011.	1.0	16
86	Flexible layered cotton cellulose-based nanofibrous membranes for piezoelectric energy harvesting and self-powered sensing. Carbohydrate Polymers, 2022, 275, 118740.	5.1	16
87	In situ formation of circular and branched oligomers in a localized high concentration electrolyte at the lithium-metal solid electrolyte interphase: a hybrid ab initio and reactive molecular dynamics study. Journal of Materials Chemistry A, 2022, 10, 632-639.	5.2	15
88	Highly Tunable Piezoelectricity of Flexible Nanogenerators Based on 3D Porously Architectured Membranes for Versatile Energy Harvesting and Self-Powered Multistimulus Sensing. ACS Sustainable Chemistry and Engineering, 2021, 9, 17128-17141.	3.2	15
89	Customizable Ligand Exchange for Tailored Surface Property of Noble Metal Nanocrystals. Research, 2020, 2020, 2131806.	2.8	13
90	Predictions of Chemical Shifts for Reactive Intermediates in CO2 Reduction under Operando Conditions. ACS Applied Materials & Interfaces, 2021, 13, 31554-31560.	4.0	12

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91	Nucleation of Graphene Layers on Magnetic Oxides: Co₃O₄(111) and Cr₂O₃(0001) from Theory and Experiment. Journal of Physical Chemistry Letters, 2017, 8, 188-192.	2.1	11
92	Reactive Molecular Dynamics Simulations to Understand Mechanical Response of Thaumasite under Temperature and Strain Rate Effects. Journal of Physical Chemistry A, 2017, 121, 4688-4697.	1.1	10
93	Reaction mechanism on Ni-C₂-NS single-atom catalysis for the efficient CO₂reduction reaction. Journal of Experimental Nanoscience, 2021, 16, 255-264.	1.3	10
94	Multiscale Simulation of Solid Electrolyte Interface Formation in Fluorinated Diluted Electrolytes with Lithium Anodes. ACS Applied Materials & Interfaces, 2022, 14, 7972-7979.	4.0	10
95	Deformation Induced Solidâ€“Solid Phase Transitions in Gamma Boron. Chemistry of Materials, 2014, 26, 4289-4298.	3.2	9
96	Prediction of the mutual solubility of water and dipropylene glycol dimethyl ether using molecular dynamics simulation. Fluid Phase Equilibria, 2012, 314, 1-6.	1.4	8
97	Reaction mechanisms and sensitivity of silicon nitrocarbamate and related systems from quantum mechanics reaction dynamics. Journal of Materials Chemistry A, 2018, 6, 5082-5097.	5.2	8
98	First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18193-18201.	3.3	7
99	Doping and temperature-dependent UV-Vis optical constants of cubic SrTiO₃: a combined spectroscopic ellipsometry and first-principles study. Optical Materials Express, 2021, 11, 895.	1.6	7
100	Bioinspired Activation of<scp>N₂</scp>on Asymmetrical Coordinated Fe Grafted<scp>1T MoS₂</scp>at Room Temperature^{â€}. Chinese Journal of Chemistry, 2021, 39, 1898-1904.	2.6	7
101	In-Silico Screening the Nitrogen Reduction Reaction on Single-Atom Electrocatalysts Anchored on MoS2. Topics in Catalysis, 2022, 65, 234-241.	1.3	7
102	In Silico Optimization of Organicâ€“Inorganic Hybrid Perovskites for Photocatalytic Hydrogen Evolution Reaction in Acidic Solution. Journal of Physical Chemistry C, 2018, 122, 20918-20922.	1.5	6
103	Ellipsometric and first-principles study on temperature-dependent UVâ€“Vis dielectric functions of GaN. Applied Optics, 2021, 60, 6869.	0.9	5
104	Reduction Mechanism of Solid Electrolyte Interphase Formation on Lithium Metal Anode: Fluorine-Rich Electrolyte. Journal of the Electrochemical Society, 2022, 169, 010503.	1.3	5
105	Theoretical Research on the Electroreduction of Carbon Dioxide. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2020, .	2.2	3
106	Insights into the pH-dependent Behavior of N-Doped Carbons for the Oxygen Reduction Reaction by First-Principles Calculations. Journal of Physical Chemistry C, 2021, 125, 26429-26436.	1.5	3
107	Temperature-dependent infrared dielectric functions and hybrid phonon-polaritons in wurtzite GaN: A spectroscopic ellipsometry and multiscale simulation study. Journal of Applied Physics, 2022, 131, .	1.1	3
108	London Dispersion Corrections to Density Functional Theory for Transition Metals Based on Fitting to Experimental Temperature-Programmed Desorption of Benzene Monolayers. Journal of Physical Chemistry Letters, 2021, 12, 73-79.	2.1	2

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109	Formation of Linear Oligomers in Solid Electrolyte Interphase via Twoâ€Electron Reduction of Ethylene Carbonate. Advanced Theory and Simulations, 2022, 5, .	1.3	2
110	Finite Temperature Ultraviolet-Visible Dielectric Functions of Tantalum Pentoxide: A Combined Spectroscopic Ellipsometry and First-Principles Study. Photonics, 2022, 9, 440.	0.9	2
111	Direct growth of graphene on dielectric substrates: Epitaxy at incommensurate and reactive interfaces. , 2016, , .		1
112	Ordered three-fold symmetric graphene oxide/buckled graphene/graphene heterostructures on MgO(111) by carbon molecular beam epitaxy. Journal of Materials Chemistry C, 2018, 6, 4225-4233.	2.7	1
113	Design of a One-Dimensional Stacked Spin Peierls System with Room-Temperature Switching from Quantum Mechanical Predictions. Journal of Physical Chemistry Letters, 2019, 10, 6432-6437.	2.1	1
114	From n-alkane to polyacetylene on Cu (110): Linkage modulation in chain growth. Science China Chemistry, 2022, 65, 733-739.	4.2	1
115	Lithium Dendrite Inhibition on Post-Charge Anode Surface: The Kinetics Role. Materials Research Society Symposia Proceedings, 2015, 1774, 31-39.	0.1	0