Karen Chan

List of Publications by Year
in descending order

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108 papers	17,024 citations	30047 54 h-index	30058 103 g-index
125 all docs	125 docs citations	125 times ranked	12934 citing authors

#	Article	IF	Citations
1	Progress and Perspectives of Electrochemical CO₂ Reduction on Copper in Aqueous Electrolyte. Chemical Reviews, 2019, 119, 7610-7672.	23.0	2,708
2	Designing an improved transition metal phosphide catalyst for hydrogen evolution using experimental and theoretical trends. Energy and Environmental Science, 2015, 8, 3022-3029.	15.6	851
3	Electrochemical Ammonia Synthesisâ€"The Selectivity Challenge. ACS Catalysis, 2017, 7, 706-709.	5.5	689
4	Promoter Effects of Alkali Metal Cations on the Electrochemical Reduction of Carbon Dioxide. Journal of the American Chemical Society, 2017, 139, 11277-11287.	6.6	653
5	Theoretical Insights into a CO Dimerization Mechanism in CO₂ Electroreduction. Journal of Physical Chemistry Letters, 2015, 6, 2032-2037.	2.1	606
6	Metal ion cycling of Cu foil for selective Câ€"C coupling in electrochemical CO2 reduction. Nature Catalysis, 2018, 1, 111-119.	16.1	600
7	Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. Nano Research, 2015, 8, 566-575.	5.8	594
8	Electrochemical Activation of CO₂ through Atomic Ordering Transformations of AuCu Nanoparticles. Journal of the American Chemical Society, 2017, 139, 8329-8336.	6.6	529
9	Understanding trends in electrochemical carbon dioxide reduction rates. Nature Communications, 2017, 8, 15438.	5.8	527
10	Understanding cation effects in electrochemical CO₂ reduction. Energy and Environmental Science, 2019, 12, 3001-3014.	15.6	433
11	Active edge sites in MoSe₂ and WSe₂ catalysts for the hydrogen evolution reaction: a density functional study. Physical Chemistry Chemical Physics, 2014, 16, 13156-13164.	1.3	426
12	Electric Field Effects in Electrochemical CO₂ Reduction. ACS Catalysis, 2016, 6, 7133-7139.	5.5	411
13	pH effects on the electrochemical reduction of CO(2) towards C2 products on stepped copper. Nature Communications, 2019, 10, 32.	5.8	371
14	Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. CheM, 2017, 3, 950-960.	5.8	326
15	Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. Surface Science, 2015, 640, 133-140.	0.8	315
16	Electrochemical Barriers Made Simple. Journal of Physical Chemistry Letters, 2015, 6, 2663-2668.	2.1	309
17	Electrochemical Carbon Monoxide Reduction on Polycrystalline Copper: Effects of Potential, Pressure, and pH on Selectivity toward Multicarbon and Oxygenated Products. ACS Catalysis, 2018, 8, 7445-7454.	5.5	305
18	Is There Anything Better than Pt for HER?. ACS Energy Letters, 2021, 6, 1175-1180.	8.8	304

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19	Machine-Learning Methods Enable Exhaustive Searches for Active Bimetallic Facets and Reveal Active Site Motifs for CO₂ Reduction. ACS Catalysis, 2017, 7, 6600-6608.	5.5	300
20	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO₂ Reduction. ChemCatChem, 2014, 6, 1899-1905.	1.8	255
21	How Doped MoS₂ Breaks Transition-Metal Scaling Relations for CO₂ Electrochemical Reduction. ACS Catalysis, 2016, 6, 4428-4437.	5.5	254
22	Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. Nature Catalysis, 2020, 3, 125-134.	16.1	252
23	CO-CO coupling on Cu facets: Coverage, strain and field effects. Surface Science, 2016, 654, 56-62.	0.8	223
24	Potential Dependence of Electrochemical Barriers from ab Initio Calculations. Journal of Physical Chemistry Letters, 2016, 7, 1686-1690.	2.1	213
25	Double layer charging driven carbon dioxide adsorption limits the rate of electrochemical carbon dioxide reduction on Gold. Nature Communications, 2020, 11, 33.	5.8	188
26	Synergistic enhancement of electrocatalytic CO2 reduction to C2 oxygenates at nitrogen-doped nanodiamonds/Cu interface. Nature Nanotechnology, 2020, 15, 131-137.	15.6	169
27	Catalytic Polysulfide Conversion and Physiochemical Confinement for Lithiumâ€“Sulfur Batteries. Advanced Energy Materials, 2020, 10, 1904010.	10.2	165
28	Unified mechanistic understanding of CO2 reduction to CO on transition metal and single atom catalysts. Nature Catalysis, 2021, 4, 1024-1031.	16.1	154
29	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. ACS Catalysis, 2019, 9, 920-931.	5.5	153
30	Rational design of MoS₂ catalysts: tuning the structure and activity via transition metal doping. Catalysis Science and Technology, 2015, 5, 246-253.	2.1	152
31	pH Effects on Hydrogen Evolution and Oxidation over Pt(111): Insights from First-Principles. ACS Catalysis, 2019, 9, 6194-6201.	5.5	136
32	Barriers of Electrochemical CO₂ Reduction on Transition Metals. Organic Process Research and Development, 2016, 20, 1424-1430.	1.3	135
33	pH in atomic scale simulations of electrochemical interfaces. Physical Chemistry Chemical Physics, 2013, 15, 10321.	1.3	127
34	Influence of Atomic Surface Structure on the Activity of Ag for the Electrochemical Reduction of CO₂ to CO. ACS Catalysis, 2019, 9, 4006-4014.	5.5	119
35	Trends in the Catalytic Activity of Hydrogen Evolution during CO₂ Electroreduction on Transition Metals. ACS Catalysis, 2018, 8, 3035-3040.	5.5	107
36	Solvation at metal/water interfaces: An ab initio molecular dynamics benchmark of common computational approaches. Journal of Chemical Physics, 2020, 152, 144703.	1.2	103

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37	Electric Field Effects in Oxygen Reduction Kinetics: Rationalizing pH Dependence at the Pt(111), Au(111), and Au(100) Electrodes. Journal of Physical Chemistry C, 2020, 124, 14581-14591.	1.5	102
38	Dipole-Field Interactions Determine the CO₂ Reduction Activity of 2D Feâ€“Nâ€“C Single-Atom Catalysts. ACS Catalysis, 2020, 10, 7826-7835.	5.5	94
39	Theoretical Investigations into Defected Graphene for Electrochemical Reduction of CO₂. ACS Sustainable Chemistry and Engineering, 2017, 5, 11080-11085.	3.2	93
40	On the pH dependence of electrochemical proton transfer barriers. Catalysis Today, 2016, 262, 36-40.	2.2	91
41	A Pore-Scale Model of Oxygen Reduction in Ionomer-Free Catalyst Layers of PEFCs. Journal of the Electrochemical Society, 2011, 158, B18.	1.3	86
42	Unified Approach to Implicit and Explicit Solvent Simulations of Electrochemical Reaction Energetics. Journal of Chemical Theory and Computation, 2019, 15, 6895-6906.	2.3	86
43	Selective reduction of CO to acetaldehyde with CuAg electrocatalysts. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 12572-12575.	3.3	85
44	Mechanistic insights into nitrogen fixation by nitrogenase enzymes. Physical Chemistry Chemical Physics, 2015, 17, 29541-29547.	1.3	84
45	2022 roadmap on low temperature electrochemical CO₂ reduction. JPhys Energy, 2022, 4, 042003.	2.3	76
46	Guiding Electrochemical Carbon Dioxide Reduction toward Carbonyls Using Copper Silver Thin Films with Interphase Miscibility. ACS Energy Letters, 2018, 3, 2947-2955.	8.8	75
47	Understanding the Reactivity of Layered Transition-Metal Sulfides: A Single Electronic Descriptor for Structure and Adsorption. Journal of Physical Chemistry Letters, 2014, 5, 3884-3889.	2.1	70
48	A few basic concepts in electrochemical carbon dioxide reduction. Nature Communications, 2020, 11, 5954.	5.8	70
49	Role of Subsurface Oxygen on Cu Surfaces for CO₂ Electrochemical Reduction. Journal of Physical Chemistry C, 2018, 122, 16209-16215.	1.5	68
50	The Predominance of Hydrogen Evolution on Transition Metal Sulfides and Phosphides under CO₂ Reduction Conditions: An Experimental and Theoretical Study. ACS Energy Letters, 2018, 3, 1450-1457.	8.8	66
51	Self-Selective Catalyst Synthesis for CO2 Reduction. Joule, 2019, 3, 1927-1936.	11.7	63
52	Solventâ€“Adsorbate Interactions and Adsorbate-Specific Solvent Structure in Carbon Dioxide Reduction on a Stepped Cu Surface. Journal of Physical Chemistry C, 2019, 123, 5999-6009.	1.5	63
53	Modeling Hydrogen Evolution Reaction Kinetics through Explicit Waterâ€“Metal Interfaces. Journal of Physical Chemistry C, 2020, 124, 28083-28092.	1.5	58
54	Theories for Electrolyte Effects in CO₂ Electroreduction. Accounts of Chemical Research, 2022, 55, 495-503.	7.6	55

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55	Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene. ACS Central Science, 2017, 3, 1286-1293.	5.3	54
56	The determination of the HOR/HER reaction mechanism from experimental kinetic data. Physical Chemistry Chemical Physics, 2021, 23, 27150-27158.	1.3	53
57	Using pH Dependence to Understand Mechanisms in Electrochemical CO Reduction. ACS Catalysis, 2022, 12, 4344-4357.	5.5	53
58	Understanding the complementarities of surface-enhanced infrared and Raman spectroscopies in CO adsorption and electrochemical reduction. Nature Communications, 2022, 13, 2656.	5.8	53
59	Understanding the Influence of [EMIM]Cl on the Suppression of the Hydrogen Evolution Reaction on Transition Metal Electrodes. Langmuir, 2017, 33, 9464-9471.	1.6	50
60	How pH affects electrochemical processes. Science, 2022, 375, 379-380.	6.0	49
61	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. Nature Communications, 2018, 9, 3202.	5.8	47
62	A Two-Dimensional MoS₂ Catalysis Transistor by Solid-State Ion Gating Manipulation and Adjustment (SIGMA). Nano Letters, 2019, 19, 7293-7300.	4.5	46
63	Computational Screening of Single and Di-Atom Catalysts for Electrochemical CO₂ Reduction. ACS Catalysis, 2022, 12, 4818-4824.	5.5	46
64	Improving the intrinsic activity of electrocatalysts for sustainable energy conversion: where are we and where can we go?. Chemical Science, 2021, 13, 14-26.	3.7	45
65	Theoretical Study of EMIM⁺ Adsorption on Silver Electrode Surfaces. Journal of Physical Chemistry C, 2015, 119, 20023-20029.	1.5	44
66	Scaling Relations on Basal Plane Vacancies of Transition Metal Dichalcogenides for CO₂ Reduction. Journal of Physical Chemistry C, 2019, 123, 4256-4261.	1.5	44
67	Practical Considerations for Continuum Models Applied to Surface Electrochemistry. ChemPhysChem, 2019, 20, 3074-3080.	1.0	40
68	Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. ACS Catalysis, 2017, 7, 2528-2534.	5.5	39
69	Fingerprint Voltammograms of Copper Single Crystals under Alkaline Conditions: A Fundamental Mechanistic Analysis. Journal of Physical Chemistry Letters, 2020, 11, 1450-1455.	2.1	38
70	Electrolyte Effects on the Stability of Niâ^'Mo Cathodes for the Hydrogen Evolution Reaction. ChemSusChem, 2019, 12, 3491-3500.	3.6	37
71	Facile Electron Transfer to CO₂ during Adsorption at the Metal|Solution Interface. Journal of Physical Chemistry C, 2019, 123, 29278-29283.	1.5	36
72	Insights into the Hydrogen Evolution Reaction on 2D Transition-Metal Dichalcogenides. Journal of Physical Chemistry C, 2022, 126, 5151-5158.	1.5	32

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73	Covalent Organic Framework (COF) Derived Niâ€Nâ€C Catalysts for Electrochemical CO₂ Reduction: Unraveling Fundamental Kinetic and Structural Parameters of the Active Sites. Angewandte Chemie - International Edition, 2022, 61, .	7.2	28
74	Local reaction environment for selective electroreduction of carbon monoxide. Energy and Environmental Science, 2022, 15, 2470-2478.	15.6	27
75	Rational design of stable sulfur vacancies in molybdenum disulfide for hydrogen evolution. Journal of Catalysis, 2020, 382, 320-328.	3.1	26
76	Preparation of open-through anodized aluminium oxide films with a clean method. Nanotechnology, 2007, 18, 245304.	1.3	25
77	Energyâ€“entropy competition in cationâ€“hydroxyl interactions at the liquid waterâ€“Pt(111) interface. Chemical Communications, 2020, 56, 427-430.	2.2	25
78	Atomistic Insight into Cation Effects on Binding Energies in Cu-Catalyzed Carbon Dioxide Reduction. Journal of Physical Chemistry C, 2020, 124, 24765-24775.	1.5	25
79	Ultrastable molybdenum disulfide-based electrocatalyst for hydrogen evolution in acidic media. Journal of Power Sources, 2020, 456, 227998.	4.0	23
80	Spin Uncoupling in Chemisorbed OCCO and CO₂: Two High-Energy Intermediates in Catalytic CO₂ Reduction. Journal of Physical Chemistry C, 2018, 122, 12251-12258.	1.5	22
81	Generalizable Trends in Electrochemical Protonation Barriers. Journal of Physical Chemistry Letters, 2021, 12, 5193-5200.	2.1	19
82	Water balance model for polymer electrolyte fuel cells with ultrathin catalyst layers. Physical Chemistry Chemical Physics, 2014, 16, 2106-2117.	1.3	18
83	Transition Metal Arsenide Catalysts for the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2019, 123, 24007-24012.	1.5	18
84	Impedance Model of Oxygen Reduction in Water-Flooded Pores of Ionomer-Free PEFC Catalyst Layers. Journal of the Electrochemical Society, 2011, 159, B155-B164.	1.3	17
85	Towards constant potential modeling of CO-CO coupling at liquid water-Cu(1 0 0) interfaces. Journal of Catalysis, 2021, 396, 251-260.	3.1	16
86	Theoretical Investigations of Transition Metal Surface Energies under Lattice Strain and CO Environment. Journal of Physical Chemistry C, 2018, 122, 14481-14487.	1.5	14
87	Understanding the reaction mechanism of Kolbe electrolysis on Pt anodes. Chem Catalysis, 2022, 2, 1100-1113.	2.9	14
88	OH Binding Energy as a Universal Descriptor of the Potential of Zero Charge on Transition Metal Surfaces. Journal of Physical Chemistry C, 2022, 126, 5521-5528.	1.5	12
89	Limits to scaling relations between adsorption energies?. Journal of Chemical Physics, 2022, 156, .	1.2	12
90	Electrochemical Oxidation of CO on Cu Single Crystals under Alkaline Conditions. ACS Energy Letters, 2020, 5, 3437-3442.	8.8	8

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91	Covalent Organic Framework (COF) Derived Niâ€Nâ€C Catalysts for Electrochemical CO₂ Reduction: Unraveling Fundamental Kinetic and Structural Parameters of the Active Sites. Angewandte Chemie, 2022, 134, .	1.6	8
92	Interaction of CO with Gold in an Electrochemical Environment. Journal of Physical Chemistry C, 2021, 125, 17684-17689.	1.5	7
93	Transients in Electrochemical CO Reduction Explained by Mass Transport of Buffers. ACS Catalysis, 2022, 12, 5155-5161.	5.5	7
94	Implications of the fractional charge of hydroxide at the electrochemical interface. Physical Chemistry Chemical Physics, 2020, 22, 6964-6969.	1.3	6
95	Force-Based Method to Determine the Potential Dependence in Electrochemical Barriers. Journal of Physical Chemistry Letters, 0, , 5719-5725.	2.1	4
96	Introduction: Computational Electrochemistry. Chemical Reviews, 2022, 122, 10579-10580.	23.0	3
97	Single Pore Modeling of Oxygen Reduction in Ionomer-Free Catalyst Layers in PEFCs. ECS Transactions, 2011, 41, 153-164.	0.3	1
98	How to extract adsorption energies, adsorbateâ€“adsorbate interaction parameters and saturation coverages from temperature programmed desorption experiments. Physical Chemistry Chemical Physics, 2021, 23, 24396-24402.	1.3	1
99	Theoretical Investigations of Electrochemical CO2 Reduction. ECS Meeting Abstracts, 2017, , .	0.0	0
100	Theoretical Investigations of Electrochemical CO2 Reduction. ECS Meeting Abstracts, 2017, , .	0.0	0
101	Effects of Introducing Metal Adatoms on the Electrochemical CO2 Reduction Behavior of Copper. ECS Meeting Abstracts, 2018, , .	0.0	0
102	Metal Ion Cycling of Cu Foil for Selective C-C Coupling in Electrochemical CO2 Reduction. ECS Meeting Abstracts, 2018, , .	0.0	0
103	Impliciations of Transport and pH Effects on Electrocatalytic CO2 Reduction. ECS Meeting Abstracts, 2018, , .	0.0	0
104	Designing Carbon-Based Materials for Effective Electrochemical Reduction of CO2. ECS Meeting Abstracts, 2018, , .	0.0	0
105	Investigation of the CO Binding Strength on CO2 to CO Catalysts using Temperature Programmed Desorption and ab initio Molecular Dynamics. , 0, , .		0
106	The electrified Cu/aqueous interface under alkaline conditions: Converging experiment and theory via kinetics. , 0, , .		0
107	Electrocatalytic Reduction of Furfural Using Single-Atom Molecular Catalysts. ECS Meeting Abstracts, 2022, MA2022-01, 961-961.	0.0	0
108	Pulsed Electrochemical CO Reduction on Mass-Selected Cu Nanoparticles. ECS Meeting Abstracts, 2022, MA2022-01, 1604-1604.	0.0	0