Karen Chan

List of Publications by Citations

91 papers	10,382 citations	46 h-index	101 g-index
125 ext. papers	13,358 ext. citations	13 avg, IF	6.84 L-index

#	Paper	IF	Citations
91	Progress and Perspectives of Electrochemical CO Reduction on Copper in Aqueous Electrolyte. *Chemical Reviews*, **2019**, 119, 7610-7672	68.1	1244
90	Designing an improved transition metal phosphide catalyst for hydrogen evolution using experimental and theoretical trends. *Energy and Environmental Science*, **2015**, 8, 3022-3029	35.4	671
89	Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. *Nano Research*, **2015**, 8, 566-575	10	478
88	Electrochemical Ammonia Synthesis□he Selectivity Challenge. *ACS Catalysis*, **2017**, 7, 706-709	13.1	442
87	Theoretical Insights into a CO Dimerization Mechanism in CO2 Electroreduction. *Journal of Physical Chemistry Letters*, **2015**, 6, 2032-7	6.4	419
86	Electrochemical Activation of CO through Atomic Ordering Transformations of AuCu Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 8329-8336	16.4	392
85	Metal ion cycling of Cu foil for selective C□ coupling in electrochemical CO2 reduction. *Nature Catalysis*, **2018**, 1, 111-119	36.5	383
84	Promoter Effects of Alkali Metal Cations on the Electrochemical Reduction of Carbon Dioxide. *Journal of the American Chemical Society*, **2017**, 139, 11277-11287	16.4	381
83	Understanding trends in electrochemical carbon dioxide reduction rates. *Nature Communications*, **2017**, 8, 15438	17.4	369
82	Active edge sites in MoSe2 and WSe2 catalysts for the hydrogen evolution reaction: a density functional study. *Physical Chemistry Chemical Physics*, **2014**, 16, 13156-64	3.6	364
81	Electric Field Effects in Electrochemical CO2 Reduction. *ACS Catalysis*, **2016**, 6, 7133-7139	13.1	275
80	Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. *Surface Science*, **2015**, 640, 133-140	1.8	256
79	Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. *CheM*, **2017**, 3, 950-960	16.2	249
78	Understanding cation effects in electrochemical CO2 reduction. *Energy and Environmental Science*, **2019**, 12, 3001-3014	35.4	231
77	Machine-Learning Methods Enable Exhaustive Searches for Active Bimetallic Facets and Reveal Active Site Motifs for CO2 Reduction. *ACS Catalysis*, **2017**, 7, 6600-6608	13.1	224
76	Electrochemical Barriers Made Simple. *Journal of Physical Chemistry Letters*, **2015**, 6, 2663-8	6.4	211
75	pH effects on the electrochemical reduction of CO towards C products on stepped copper. *Nature Communications*, **2019**, 10, 32	17.4	207

74	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO2 Reduction. *ChemCatChem*, **2014**, 6, 1899-1905	5.2	194
73	How Doped MoS2 Breaks Transition-Metal Scaling Relations for CO2 Electrochemical Reduction. *ACS Catalysis*, **2016**, 6, 4428-4437	13.1	193
72	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	13.1	175
71	CO-CO coupling on Cu facets: Coverage, strain and field effects. *Surface Science*, **2016**, 654, 56-62	1.8	142
70	Potential Dependence of Electrochemical Barriers from ab Initio Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 1686-90	6.4	138
69	Rational design of MoS2 catalysts: tuning the structure and activity via transition metal doping. *Catalysis Science and Technology*, **2015**, 5, 246-253	5.5	128
68	Double layer charging driven carbon dioxide adsorption limits the rate of electrochemical carbon dioxide reduction on Gold. *Nature Communications*, **2020**, 11, 33	17.4	107
67	Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. *Nature Catalysis*, **2020**, 3, 125-134	36.5	106
66	pH in atomic scale simulations of electrochemical interfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 10321-5	3.6	100
65	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. *ACS Catalysis*, **2019**, 9, 920-931	13.1	100
64	Barriers of Electrochemical CO2 Reduction on Transition Metals. *Organic Process Research and Development*, **2016**, 20, 1424-1430	3.9	98
63	Catalytic Polysulfide Conversion and Physiochemical Confinement for Lithium–Sulfur Batteries. *Advanced Energy Materials*, **2020**, 10, 1904010	21.8	94
62	Synergistic enhancement of electrocatalytic CO reduction to C oxygenates at nitrogen-doped nanodiamonds/Cu interface. *Nature Nanotechnology*, **2020**, 15, 131-137	28.7	92
61	Is There Anything Better than Pt for HER?. *ACS Energy Letters*, **2021**, 6, 1175-1180	20.1	83
60	A Pore-Scale Model of Oxygen Reduction in Ionomer-Free Catalyst Layers of PEFCs. *Journal of the Electrochemical Society*, **2011**, 158, B18	3.9	73
59	Influence of Atomic Surface Structure on the Activity of Ag for the Electrochemical Reduction of CO2 to CO. *ACS Catalysis*, **2019**, 9, 4006-4014	13.1	72
58	Theoretical Investigations into Defected Graphene for Electrochemical Reduction of CO2. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 11080-11085	8.3	68
57	On the pH dependence of electrochemical proton transfer barriers. *Catalysis Today*, **2016**, 262, 36-40	5.3	68

56	Trends in the Catalytic Activity of Hydrogen Evolution during CO2 Electroreduction on Transition Metals. *ACS Catalysis*, **2018**, 8, 3035-3040	13.1	67
55	pH Effects on Hydrogen Evolution and Oxidation over Pt(111): Insights from First-Principles. *ACS Catalysis*, **2019**, 9, 6194-6201	13.1	64
54	Mechanistic insights into nitrogen fixation by nitrogenase enzymes. *Physical Chemistry Chemical Physics*, **2015**, 17, 29541-7	3.6	62
53	Understanding the Reactivity of Layered Transition-Metal Sulfides: A Single Electronic Descriptor for Structure and Adsorption. *Journal of Physical Chemistry Letters*, **2014**, 5, 3884-9	6.4	57
52	Solvation at metal/water interfaces: An ab initio molecular dynamics benchmark of common computational approaches. *Journal of Chemical Physics*, **2020**, 152, 144703	3.9	56
51	Unified Approach to Implicit and Explicit Solvent Simulations of Electrochemical Reaction Energetics. *Journal of Chemical Theory and Computation*, **2019**, 15, 6895-6906	6.4	51
50	Role of Subsurface Oxygen on Cu Surfaces for CO2 Electrochemical Reduction. *Journal of Physical Chemistry C*, **2018**, 122, 16209-16215	3.8	49
49	Dipole-Field Interactions Determine the CO2 Reduction Activity of 2D Fe□□ Single-Atom Catalysts. *ACS Catalysis*, **2020**, 10, 7826-7835	13.1	48
48	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	20.1	48
47	Guiding Electrochemical Carbon Dioxide Reduction toward Carbonyls Using Copper Silver Thin Films with Interphase Miscibility. *ACS Energy Letters*, **2018**, 3, 2947-2955	20.1	47
46	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	3.8	44
45	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	11.5	43
44	Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene. *ACS Central Science*, **2017**, 3, 1286-1293	16.8	41
43	Solvent□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	3.8	39
42	Understanding the Influence of [EMIM]Cl on the Suppression of the Hydrogen Evolution Reaction on Transition Metal Electrodes. *Langmuir*, **2017**, 33, 9464-9471	4	36
41	Self-Selective Catalyst Synthesis for CO2 Reduction. *Joule*, **2019**, 3, 1927-1936	27.8	35
40	Theoretical Study of EMIM+ Adsorption on Silver Electrode Surfaces. *Journal of Physical Chemistry C* , **2015**, 119, 20023-20029	3.8	33
39	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. *Nature Communications*, **2018**, 9, 3202	17.4	31

38	Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. *ACS Catalysis*, **2017**, 7, 2528-2534	13.1	30
37	A few basic concepts in electrochemical carbon dioxide reduction. *Nature Communications*, **2020**, 11, 5954	17.4	30
36	Unified mechanistic understanding of CO2 reduction to CO on transition metal and single atom catalysts. *Nature Catalysis*,	36.5	29
35	Scaling Relations on Basal Plane Vacancies of Transition Metal Dichalcogenides for CO2 Reduction. *Journal of Physical Chemistry C*, **2019**, 123, 4256-4261	3.8	28
34	A Two-Dimensional MoS Catalysis Transistor by Solid-State Ion Gating Manipulation and Adjustment (SIGMA). *Nano Letters*, **2019**, 19, 7293-7300	11.5	24
33	Modeling Hydrogen Evolution Reaction Kinetics through Explicit Water|Metal Interfaces. *Journal of Physical Chemistry C*, **2020**, 124, 28083-28092	3.8	24
32	Fingerprint Voltammograms of Copper Single Crystals under Alkaline Conditions: A Fundamental Mechanistic Analysis. *Journal of Physical Chemistry Letters*, **2020**, 11, 1450-1455	6.4	23
31	Facile Electron Transfer to CO2 during Adsorption at the Metal|Solution Interface. *Journal of Physical Chemistry C*, **2019**, 123, 29278-29283	3.8	23
30	Practical Considerations for Continuum Models Applied to Surface Electrochemistry. *ChemPhysChem*, **2019**, 20, 3074-3080	3.2	21
29	Electrolyte Effects on the Stability of Ni-Mo Cathodes for the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 3491-3500	8.3	20
28	Preparation of open-through anodized aluminium oxide films with a clean method. *Nanotechnology* , **2007**, 18, 245304	3.4	20
27	Energy-entropy competition in cation-hydroxyl interactions at the liquid water-Pt(111) interface. *Chemical Communications*, **2020**, 56, 427-430	5.8	17
26	Rational design of stable sulfur vacancies in molybdenum disulfide for hydrogen evolution. *Journal of Catalysis*, **2020**, 382, 320-328	7.3	15
25	Ultrastable molybdenum disulfide-based electrocatalyst for hydrogen evolution in acidic media. *Journal of Power Sources*, **2020**, 456, 227998	8.9	13
24	Water balance model for polymer electrolyte fuel cells with ultrathin catalyst layers. *Physical Chemistry Chemical Physics*, **2014**, 16, 2106-17	3.6	13
23	Atomistic Insight into Cation Effects on Binding Energies in Cu-Catalyzed Carbon Dioxide Reduction. *Journal of Physical Chemistry C*, **2020**, 124, 24765-24775	3.8	12
22	Spin Uncoupling in Chemisorbed OCCO and CO2: Two High-Energy Intermediates in Catalytic CO2 Reduction. *Journal of Physical Chemistry C*, **2018**, 122, 12251-12258	3.8	12
21	Impedance Model of Oxygen Reduction in Water-Flooded Pores of Ionomer-Free PEFC Catalyst Layers. *Journal of the Electrochemical Society*, **2011**, 159, B155-B164	3.9	12

20	Theoretical Investigations of Transition Metal Surface Energies under Lattice Strain and CO Environment. *Journal of Physical Chemistry C*, **2018**, 122, 14481-14487	3.8	12
19	Improving the intrinsic activity of electrocatalysts for sustainable energy conversion: where are we and where can we go?. *Chemical Science*, **2021**, 13, 14-26	9.4	11
18	Generalizable Trends in Electrochemical Protonation Barriers. *Journal of Physical Chemistry Letters*, **2021**, 12, 5193-5200	6.4	11
17	The determination of the HOR/HER reaction mechanism from experimental kinetic data. *Physical Chemistry Chemical Physics*, **2021**,	3.6	6
16	Electrochemical Oxidation of CO on Cu Single Crystals under Alkaline Conditions. *ACS Energy Letters*, **2020**, 5, 3437-3442	20.1	6
15	Insights into the Hydrogen Evolution Reaction on 2D Transition-Metal Dichalcogenides. *Journal of Physical Chemistry C*, **2022**, 126, 5151-5158	3.8	6
14	Using pH Dependence to Understand Mechanisms in Electrochemical CO Reduction. *ACS Catalysis*,4344-4357	13.7	6
13	Implications of the fractional charge of hydroxide at the electrochemical interface. *Physical Chemistry Chemical Physics*, **2020**, 22, 6964-6969	3.6	5
12	How pH affects electrochemical processes.. *Science*, **2022**, 375, 379-380	33.3	5
11	Computational Screening of Single and Di-Atom Catalysts for Electrochemical CO2 Reduction. *ACS Catalysis*,4818-4824	13.1	5
10	Understanding the complementarities of surface-enhanced infrared and Raman spectroscopies in CO adsorption and electrochemical reduction.. *Nature Communications*, **2022**, 13, 2656	17.4	5
9	Transition Metal Arsenide Catalysts for the Hydrogen Evolution Reaction. *Journal of Physical Chemistry C*, **2019**, 123, 24007-24012	3.8	4
8	Towards constant potential modeling of CO-CO coupling at liquid water-Cu(1 0 0) interfaces. *Journal of Catalysis*, **2021**, 396, 251-260	7.3	4
7	Mechanism for acetate formation in CO(2) reduction on Cu: Selectivity trends with pH and nanostructuring derive from mass transport		3
6	Interaction of CO with Gold in an Electrochemical Environment. *Journal of Physical Chemistry C*, **2021**, 125, 17684-17689	3.8	3
5	Transients in Electrochemical CO Reduction Explained by Mass Transport of Buffers. *ACS Catalysis*,5155-5161	13.1	3
4	Understanding the reaction mechanism of Kolbe electrolysis on Pt anodes. *Chem Catalysis*, **2022**,		2
3	How to extract adsorption energies, adsorbate-adsorbate interaction parameters and saturation coverages from temperature programmed desorption experiments. *Physical Chemistry Chemical Physics*, **2021**, 23, 24396-24402	3.6	1

2	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	3.8	1
1	Nanoscale Phenomena in Catalyst Layers for PEM Fuel Cells: From Fundamental Physics to Benign Design **2010**, 317-369		