# Karen Chan

## List of Publications by Year in Descending Order



| | | | |
|---|---|---|---|
| 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 | How pH affects electrochemical processes.. *Science*, **2022**, 375, 379-380 | 33.3 | 5 |
| 90 | Understanding the reaction mechanism of Kolbe electrolysis on Pt anodes. *Chem Catalysis*, **2022**, | | 2 |
| 89 | 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 |
| 88 | Insights into the Hydrogen Evolution Reaction on 2D Transition-Metal Dichalcogenides. *Journal of Physical Chemistry C*, **2022**, 126, 5151-5158 | 3.8 | 6 |
| 87 | Understanding the complementarities of surface-enhanced infrared and Raman spectroscopies in CO adsorption and electrochemical reduction.. *Nature Communications*, **2022**, 13, 2656 | 17.4 | 5 |
| 86 | 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 |
| 85 | The determination of the HOR/HER reaction mechanism from experimental kinetic data. *Physical Chemistry Chemical Physics*, **2021**, | 3.6 | 6 |
| 84 | 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 |
| 83 | Is There Anything Better than Pt for HER?. *ACS Energy Letters*, **2021**, 6, 1175-1180 | 20.1 | 83 |
| 82 | 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 |
| 81 | Generalizable Trends in Electrochemical Protonation Barriers. *Journal of Physical Chemistry Letters*, **2021**, 12, 5193-5200 | 6.4 | 11 |
| 80 | Interaction of CO with Gold in an Electrochemical Environment. *Journal of Physical Chemistry C*, **2021**, 125, 17684-17689 | 3.8 | 3 |
| 79 | 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 |
| 78 | 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 |
| 77 | Dipole-Field Interactions Determine the CO2 Reduction Activity of 2D Fe□□ Single-Atom Catalysts. *ACS Catalysis*, **2020**, 10, 7826-7835 | 13.1 | 48 |
| 76 | Implications of the fractional charge of hydroxide at the electrochemical interface. *Physical Chemistry Chemical Physics*, **2020**, 22, 6964-6969 | 3.6 | 5 |
| 75 | Rational design of stable sulfur vacancies in molybdenum disulfide for hydrogen evolution. *Journal of Catalysis*, **2020**, 382, 320-328 | 7.3 | 15 |

| | | | |
|---|---|---|---|
| 74 | 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 |
| 73 | 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 |
| 72 | 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 |
| 71 | Catalytic Polysulfide Conversion and Physiochemical Confinement for Lithium–Sulfur Batteries. *Advanced Energy Materials*, **2020**, 10, 1904010 | 21.8 | 94 |
| 70 | Ultrastable molybdenum disulfide-based electrocatalyst for hydrogen evolution in acidic media. *Journal of Power Sources*, **2020**, 456, 227998 | 8.9 | 13 |
| 69 | Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. *Nature Catalysis*, **2020**, 3, 125-134 | 36.5 | 106 |
| 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 | Energy-entropy competition in cation-hydroxyl interactions at the liquid water-Pt(111) interface. *Chemical Communications*, **2020**, 56, 427-430 | 5.8 | 17 |
| 66 | Synergistic enhancement of electrocatalytic CO reduction to C oxygenates at nitrogen-doped nanodiamonds/Cu interface. *Nature Nanotechnology*, **2020**, 15, 131-137 | 28.7 | 92 |
| 65 | Electrochemical Oxidation of CO on Cu Single Crystals under Alkaline Conditions. *ACS Energy Letters*, **2020**, 5, 3437-3442 | 20.1 | 6 |
| 64 | A few basic concepts in electrochemical carbon dioxide reduction. *Nature Communications*, **2020**, 11, 5954 | 17.4 | 30 |
| 63 | Modeling Hydrogen Evolution Reaction Kinetics through Explicit Water–Metal Interfaces. *Journal of Physical Chemistry C*, **2020**, 124, 28083-28092 | 3.8 | 24 |
| 62 | A Two-Dimensional MoS Catalysis Transistor by Solid-State Ion Gating Manipulation and Adjustment (SIGMA). *Nano Letters*, **2019**, 19, 7293-7300 | 11.5 | 24 |
| 61 | Transition Metal Arsenide Catalysts for the Hydrogen Evolution Reaction. *Journal of Physical Chemistry C*, **2019**, 123, 24007-24012 | 3.8 | 4 |
| 60 | 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 |
| 59 | Progress and Perspectives of Electrochemical CO Reduction on Copper in Aqueous Electrolyte. *Chemical Reviews*, **2019**, 119, 7610-7672 | 68.1 | 1244 |
| 58 | pH Effects on Hydrogen Evolution and Oxidation over Pt(111): Insights from First-Principles. *ACS Catalysis*, **2019**, 9, 6194-6201 | 13.1 | 64 |
| 57 | Electrolyte Effects on the Stability of Ni-Mo Cathodes for the Hydrogen Evolution Reaction. *ChemSusChem*, **2019**, 12, 3491-3500 | 8.3 | 20 |

| | | | |
|---|---|---|---|
| 56 | 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 |
| 55 | Practical Considerations for Continuum Models Applied to Surface Electrochemistry. *ChemPhysChem*, **2019**, 20, 3074-3080 | 3.2 | 21 |
| 54 | Understanding cation effects in electrochemical CO2 reduction. *Energy and Environmental Science*, **2019**, 12, 3001-3014 | 35.4 | 231 |
| 53 | Self-Selective Catalyst Synthesis for CO2 Reduction. *Joule*, **2019**, 3, 1927-1936 | 27.8 | 35 |
| 52 | 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 |
| 51 | Facile Electron Transfer to CO2 during Adsorption at the Metal\|Solution Interface. *Journal of Physical Chemistry C*, **2019**, 123, 29278-29283 | 3.8 | 23 |
| 50 | 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 |
| 49 | pH effects on the electrochemical reduction of CO towards C products on stepped copper. *Nature Communications*, **2019**, 10, 32 | 17.4 | 207 |
| 48 | Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. *ACS Catalysis*, **2019**, 9, 920-931 | 13.1 | 100 |
| 47 | Trends in the Catalytic Activity of Hydrogen Evolution during CO2 Electroreduction on Transition Metals. *ACS Catalysis*, **2018**, 8, 3035-3040 | 13.1 | 67 |
| 46 | Metal ion cycling of Cu foil for selective C–C coupling in electrochemical CO2 reduction. *Nature Catalysis*, **2018**, 1, 111-119 | 36.5 | 383 |
| 45 | 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 |
| 44 | 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 |
| 43 | Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. *Nature Communications*, **2018**, 9, 3202 | 17.4 | 31 |
| 42 | Role of Subsurface Oxygen on Cu Surfaces for CO2 Electrochemical Reduction. *Journal of Physical Chemistry C*, **2018**, 122, 16209-16215 | 3.8 | 49 |
| 41 | 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 |
| 40 | 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 |
| 39 | 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 |

| | | | |
|---|---|---|---|
| 38 | Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. *ACS Catalysis*, **2017**, 7, 2528-2534 | 13.1 | 30 |
| 37 | Understanding trends in electrochemical carbon dioxide reduction rates. *Nature Communications*, **2017**, 8, 15438 | 17.4 | 369 |
| 36 | Electrochemical Activation of CO through Atomic Ordering Transformations of AuCu Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 8329-8336 | 16.4 | 392 |
| 35 | Electrochemical Ammonia Synthesis□he Selectivity Challenge. *ACS Catalysis*, **2017**, 7, 706-709 | 13.1 | 442 |
| 34 | Theoretical Investigations into Defected Graphene for Electrochemical Reduction of CO2. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 11080-11085 | 8.3 | 68 |
| 33 | Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. *CheM*, **2017**, 3, 950-960 | 16.2 | 249 |
| 32 | 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 |
| 31 | 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 |
| 30 | 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 |
| 29 | 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 |
| 28 | Barriers of Electrochemical CO2 Reduction on Transition Metals. *Organic Process Research and Development*, **2016**, 20, 1424-1430 | 3.9 | 98 |
| 27 | How Doped MoS2 Breaks Transition-Metal Scaling Relations for CO2 Electrochemical Reduction. *ACS Catalysis*, **2016**, 6, 4428-4437 | 13.1 | 193 |
| 26 | On the pH dependence of electrochemical proton transfer barriers. *Catalysis Today*, **2016**, 262, 36-40 | 5.3 | 68 |
| 25 | Potential Dependence of Electrochemical Barriers from ab Initio Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 1686-90 | 6.4 | 138 |
| 24 | CO-CO coupling on Cu facets: Coverage, strain and field effects. *Surface Science*, **2016**, 654, 56-62 | 1.8 | 142 |
| 23 | Electric Field Effects in Electrochemical CO2 Reduction. *ACS Catalysis*, **2016**, 6, 7133-7139 | 13.1 | 275 |
| 22 | Electrochemical Barriers Made Simple. *Journal of Physical Chemistry Letters*, **2015**, 6, 2663-8 | 6.4 | 211 |
| 21 | Theoretical Insights into a CO Dimerization Mechanism in CO2 Electroreduction. *Journal of Physical Chemistry Letters*, **2015**, 6, 2032-7 | 6.4 | 419 |

| | | | |
|---|---|---|---|
| 20 | Mechanistic insights into nitrogen fixation by nitrogenase enzymes. *Physical Chemistry Chemical Physics*, **2015**, 17, 29541-7 | 3.6 | 62 |
| 19 | 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 |
| 18 | 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 |
| 17 | Theoretical Study of EMIM+ Adsorption on Silver Electrode Surfaces. *Journal of Physical Chemistry C* , **2015**, 119, 20023-20029 | 3.8 | 33 |
| 16 | Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. *Surface Science*, **2015**, 640, 133-140 | 1.8 | 256 |
| 15 | Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. *Nano Research*, **2015**, 8, 566-575 | 10 | 478 |
| 14 | 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 |
| 13 | Water balance model for polymer electrolyte fuel cells with ultrathin catalyst layers. *Physical Chemistry Chemical Physics*, **2014**, 16, 2106-17 | 3.6 | 13 |
| 12 | 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 |
| 11 | Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO2 Reduction. *ChemCatChem*, **2014**, 6, 1899-1905 | 5.2 | 194 |
| 10 | pH in atomic scale simulations of electrochemical interfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 10321-5 | 3.6 | 100 |
| 9 | 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 |
| 8 | 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 |
| 7 | Nanoscale Phenomena in Catalyst Layers for PEM Fuel Cells: From Fundamental Physics to Benign Design **2010**, 317-369 | | |
| 6 | Preparation of open-through anodized aluminium oxide films with a clean method. *Nanotechnology* , **2007**, 18, 245304 | 3.4 | 20 |
| 5 | Unified mechanistic understanding of CO2 reduction to CO on transition metal and single atom catalysts. *Nature Catalysis*, | 36.5 | 29 |
| 4 | Mechanism for acetate formation in CO(2) reduction on Cu: Selectivity trends with pH and nanostructuring derive from mass transport | | 3 |
| 3 | Using pH Dependence to Understand Mechanisms in Electrochemical CO Reduction. *ACS Catalysis*,4344-4357 | 13.1 | 6 |

| | | | |
|---|---|---|---|
| 2 | Computational Screening of Single and Di-Atom Catalysts for Electrochemical CO2 Reduction. *ACS Catalysis*,4818-4824 | 13.1 | 5 |
| 1 | Transients in Electrochemical CO Reduction Explained by Mass Transport of Buffers. *ACS Catalysis*,5155-5161 | 13.1 | 3 |