Andrew A Peterson

List of Publications by Year
in descending order

52 papers	13,926 citations	109321 35 h-index	168389 53 g-index
54 all docs	54 docs citations	54 times ranked	14921 citing authors

#	Article	IF	Citations
1	A nearsighted force-training approach to systematically generate training data for the machine learning of large atomic structures. Journal of Chemical Physics, 2022, 156, 064104.	3.0	5
2	Sulfur promotes hydrogen evolution on molybdenum carbide catalysts. Materials Advances, 2021, 2, 4867-4875.	5.4	7
3	Training sets based on uncertainty estimates in the cluster-expansion method. JPhys Energy, 2021, 3, 034012.	5.3	7
4	Heterogeneity in susceptibility dictates the order of epidemic models. Journal of Theoretical Biology, 2021, 528, 110839.	1.7	14
5	A Challenge to the <i>G</i> âˆ¼ 0 Interpretation of Hydrogen Evolution. ACS Catalysis, 2020, 10, 121-128.	11.2	166
6	Anisotropic Strain Tuning of L1₀ Ternary Nanoparticles for Oxygen Reduction. Journal of the American Chemical Society, 2020, 142, 19209-19216.	13.7	76
7	On the Coupling of Electron Transfer to Proton Transfer at Electrified Interfaces. Journal of the American Chemical Society, 2020, 142, 11829-11834.	13.7	29
8	The Electrochemical Mechanisms of Solidâ€“Electrolyte Interphase Formation in Lithium-Based Batteries. Journal of Physical Chemistry C, 2019, 123, 20084-20092.	3.1	19
9	Scaled and Dynamic Optimizations of Nudged Elastic Bands. Journal of Chemical Theory and Computation, 2019, 15, 5787-5793.	5.3	20
10	Strain-induced changes to the methanation reaction on thin-film nickel catalysts. Catalysis Science and Technology, 2019, 9, 3279-3286.	4.1	4
11	Cu nanowire-catalyzed electrochemical reduction of CO or CO₂. Nanoscale, 2019, 11, 12075-12079.	5.6	43
12	Hard-Magnet L10-CoPt Nanoparticles Advance Fuel Cell Catalysis. Joule, 2019, 3, 124-135.	24.0	326
13	Face-centered tetragonal (FCT) Fe and Co alloys of Pt as catalysts for the oxygen reduction reaction (ORR): A DFT study. Journal of Chemical Physics, 2019, 150, 041704.	3.0	29
14	The role of oxygen vacancies in biomass deoxygenation by reducible zinc/zinc oxide catalysts. Catalysis Science and Technology, 2018, 8, 1819-1827.	4.1	33
15	How strain can break the scaling relations of catalysis. Nature Catalysis, 2018, 1, 263-268.	34.4	261
16	Nanocomposites of transition-metal carbides on reduced graphite oxide as catalysts for the hydrogen evolution reaction. Applied Catalysis B: Environmental, 2018, 235, 36-44.	20.2	88
17	The potential for machine learning in hybrid QM/MM calculations. Journal of Chemical Physics, 2018, 148, 241740.	3.0	39
18	Controlled-Potential Simulation of Elementary Electrochemical Reactions: Proton Discharge on Metal Surfaces. Journal of Physical Chemistry C, 2018, 122, 12771-12781.	3.1	120

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19	Addressing uncertainty in atomistic machine learning. Physical Chemistry Chemical Physics, 2017, 19, 10978-10985.	2.8	128
20	The atomic simulation environmentâ€"a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
21	Oxidation suppression during hydrothermal phase reversion allows synthesis of monolayer semiconducting MoS₂ in stable aqueous suspension. Nanoscale, 2017, 9, 5398-5403.	5.6	36
22	High Elastic Strain Directly Tunes the Hydrogen Evolution Reaction on Tungsten Carbide. Journal of Physical Chemistry C, 2017, 121, 6177-6183.	3.1	50
23	The Influence of Elastic Strain on Catalytic Activity in the Hydrogen Evolution Reaction. Angewandte Chemie, 2016, 128, 6283-6289.	2.0	22
24	The Influence of Elastic Strain on Catalytic Activity in the Hydrogen Evolution Reaction. Angewandte Chemie - International Edition, 2016, 55, 6175-6181.	13.8	133
25	Acceleration of saddle-point searches with machine learning. Journal of Chemical Physics, 2016, 145, 074106.	3.0	125
26	Operando Raman Spectroscopy of Amorphous Molybdenum Sulfide (MoS_{<i>x</i>}) during the Electrochemical Hydrogen Evolution Reaction: Identification of Sulfur Atoms as Catalytically Active Sites for H⁺ Reduction. ACS Catalysis, 2016, 6, 7790-7798.	11.2	210
27	Amp: A modular approach to machine learning in atomistic simulations. Computer Physics Communications, 2016, 207, 310-324.	7.5	281
28	Understanding the Low-Overpotential Production of CH₄ from CO₂ on Mo₂C Catalysts. ACS Catalysis, 2016, 6, 2003-2013.	11.2	80
29	Catalytic Activities of Sulfur Atoms in Amorphous Molybdenum Sulfide for the Electrochemical Hydrogen Evolution Reaction. ACS Catalysis, 2016, 6, 861-867.	11.2	280
30	Design Principles for Metal Oxide Redox Materials for Solarâ€Driven Isothermal Fuel Production. Advanced Energy Materials, 2015, 5, 1401082.	19.5	52
31	Oxygen-induced changes to selectivity-determining steps in electrocatalytic CO₂ reduction. Physical Chemistry Chemical Physics, 2015, 17, 4505-4515.	2.8	43
32	Role of Elastic Strain on Electrocatalysis of Oxygen Reduction Reaction on Pt. Journal of Physical Chemistry C, 2015, 119, 19042-19052.	3.1	40
33	Elastic strain effects on catalysis of a PdCuSi metallic glass thin film. Physical Chemistry Chemical Physics, 2015, 17, 1746-1754.	2.8	26
34	Global Optimization of Adsorbateâ€"Surface Structures While Preserving Molecular Identity. Topics in Catalysis, 2014, 57, 40-53.	2.8	67
35	Active and Selective Conversion of CO₂ to CO on Ultrathin Au Nanowires. Journal of the American Chemical Society, 2014, 136, 16132-16135.	13.7	784
36	Looped-oxide catalysis: a solar thermal approach to bio-oil deoxygenation. Energy and Environmental Science, 2014, 7, 3122-3134.	30.8	25

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37	Departures from the Adsorption Energy Scaling Relations for Metal Carbide Catalysts. Journal of Physical Chemistry C, 2014, 118, 13026-13034.	3.1	108
38	Competition between CO₂ Reduction and H₂ Evolution on Transition-Metal Electrocatalysts. ACS Catalysis, 2014, 4, 3742-3748.	11.2	378
39	Understanding Strain and Ligand Effects in Hydrogen Evolution over Pd(111) Surfaces. Journal of Physical Chemistry C, 2014, 118, 4275-4281.	3.1	99
40	Trends in the Hydrogen Evolution Activity of Metal Carbide Catalysts. ACS Catalysis, 2014, 4, 1274-1278.	11.2	351
41	Electroreduction of Methanediol on Copper. Catalysis Letters, 2013, 143, 631-635.	2.6	21
42	Understanding Trends in the Electrocatalytic Activity of Metals and Enzymes for CO₂ Reduction to CO. Journal of Physical Chemistry Letters, 2013, 4, 388-392.	4.6	604
43	Insights into Cï£¿C Coupling in CO₂ Electroreduction on Copper Electrodes. ChemCatChem, 2013, 5, 737-742.	3.7	339
44	Catalysis in supercritical water: Pathway of the methanation reaction and sulfur poisoning over a Ru/C catalyst during the reforming of biomolecules. Journal of Catalysis, 2013, 301, 38-45.	6.2	55
45	Finite-Size Effects in O and CO Adsorption for the Late Transition Metals. Topics in Catalysis, 2012, 55, 1276-1282.	2.8	68
46	Activity Descriptors for CO₂ Electroreduction to Methane on Transition-Metal Catalysts. Journal of Physical Chemistry Letters, 2012, 3, 251-258.	4.6	1,250
47	Evidence of Scrambling over Rutheniumâ€based Catalysts in Supercriticalâ€water Gasification. ChemCatChem, 2012, 4, 1185-1189.	3.7	21
48	Production of C₃ Hydrocarbons from Biomass via Hydrothermal Carboxylate Reforming. Industrial & Engineering Chemistry Research, 2011, 50, 4420-4424.	3.7	18
49	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. Surface Science, 2011, 605, 1354-1359.	1.9	445
50	How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. Energy and Environmental Science, 2010, 3, 1311.	30.8	2,682
51	Kinetic Evidence of the Maillard Reaction in Hydrothermal Biomass Processing: Glucoseâˆ'Glycine Interactions in High-Temperature, High-Pressure Water. Industrial & Engineering Chemistry Research, 2010, 49, 2107-2117.	3.7	161
52	Thermochemical biofuel production in hydrothermal media: A review of sub- and supercritical water technologies. Energy and Environmental Science, 2008, 1, 32.	30.8	1,709