Kathleen A Schwarz

List of Publications by Year
in descending order

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27 papers	1,622 citations	430874 18 h-index	526287 27 g-index
28 all docs	28 docs citations	28 times ranked	2442 citing authors

#	Article	IF	Citations
1	Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of Battery Electrode and Electrolyte. Nano Letters, 2014, 14, 1453-1459.	9.1	238
2	JDFTx: Software for joint density-functional theory. SoftwareX, 2017, 6, 278-284.	2.6	238
3	Coâ€adsorption of Cations as the Cause of the Apparent pH Dependence of Hydrogen Adsorption on a Stepped Platinum Singleâ€Crystal Electrode. Angewandte Chemie - International Edition, 2017, 56, 15025-15029.	13.8	221
4	The importance of nonlinear fluid response in joint density-functional theory studies of battery systems. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 074005.	2.0	177
5	Direct visualization of sulfur cathodes: new insights into Liâ€“S batteries via operando X-ray based methods. Energy and Environmental Science, 2018, 11, 202-210.	30.8	96
6	The electrochemical interface in first-principles calculations. Surface Science Reports, 2020, 75, 100492.	7.2	89
7	Evaluating continuum solvation models for the electrode-electrolyte interface: Challenges and strategies for improvement. Journal of Chemical Physics, 2017, 146, 084111.	3.0	79
8	Formic acid oxidation on platinum: a simple mechanistic study. Physical Chemistry Chemical Physics, 2015, 17, 20805-20813.	2.8	56
9	Effect of Step Density and Orientation on the Apparent pH Dependence of Hydrogen and Hydroxide Adsorption on Stepped Platinum Surfaces. Journal of Physical Chemistry C, 2018, 122, 16756-16764.	3.1	50
10	Spicing up continuum solvation models with SaLSA: The spherically averaged liquid susceptibility ansatz. Journal of Chemical Physics, 2015, 142, 054102.	3.0	48
11	Partial oxidation of step-bound water leads to anomalous pH effects on metal electrode step-edges. Physical Chemistry Chemical Physics, 2016, 18, 16216-16223.	2.8	40
12	Improving the Accuracy of Atomistic Simulations of the Electrochemical Interface. Chemical Reviews, 2022, 122, 10651-10674.	47.7	39
13	Improving accuracy of electrochemical capacitance and solvation energetics in first-principles calculations. Journal of Chemical Physics, 2018, 148, 144105.	3.0	37
14	Coâ€adsorption of Cations as the Cause of the Apparent pH Dependence of Hydrogen Adsorption on a Stepped Platinum Singleâ€Crystal Electrode. Angewandte Chemie, 2017, 129, 15221-15225.	2.0	34
15	Absence of diffuse double layer effect on the vibrational properties and oxidation of chemisorbed carbon monoxide on a Pt(111) electrode. Electrochimica Acta, 2018, 281, 127-132.	5.2	31
16	Electrochemical Capacitance of CO-Terminated Pt(111) Dominated by the COâ€“Solvent Gap. Journal of Physical Chemistry Letters, 2017, 8, 5344-5348.	4.6	30
17	Spectroscopic Characterization of Charged Defects in Polycrystalline Pentacene by Timeâ€and Wavelengthâ€Resolved Electric Force Microscopy. Advanced Materials, 2011, 23, 624-628.	21.0	26
18	Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2021, 125, 154-164.	2.5	24

#	Article	IF	Citations
19	Framework for solvation in quantum Monte Carlo. Physical Review B, 2012, 85, .	3.2	14
20	Halide-Induced Step Faceting and Dissolution Energetics from Atomistic Machine Learned Potentials on Cu(100). Journal of Physical Chemistry C, 2020, 124, 12359-12369.	3.1	13
21	Measuring ion-pairing and hydration in variable charge supramolecular cages with microwave microfluidics. Communications Chemistry, 2019, 2, .	4.5	12
22	Interfacial water asymmetry at ideal electrochemical interfaces. Journal of Chemical Physics, 2022, 156, 014705.	3.0	12
23	Site-specific experiments on folding/unfolding of Jun coiled coils: Thermodynamic and kinetic parameters from spin inversion transfer nuclear magnetic resonance at leucine-18. Biopolymers, 2006, 83, 255-267.	2.4	8
24	Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of a Battery Electrode and Electrolyte. Microscopy and Microanalysis, 2014, 20, 1524-1525.	0.4	2
25	Computationally efficient dielectric calculations of molecular crystals. Journal of Chemical Physics, 2015, 142, 214101.	3.0	2
26	Resolving the Geometry/Charge Puzzle of the c(2 Ã— 2)-Cl Cu(100) Electrode. Journal of Physical Chemistry Letters, 2021, 12, 440-446.	4.6	2
27	Compressive Stress and Charge Redistribution during CO Adsorption onto Pt. Journal of Physical Chemistry C, 2022, 126, 4446-4457.	3.1	0