

Tod A Pascal

List of Publications by Year in descending order

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46
papers

2,989
citations

218677

26
h-index

233421

45
g-index

47
all docs

47
docs citations

47
times ranked

4250
citing authors

#	ARTICLE	IF	CITATIONS
1	The structure of interfacial water on gold electrodes studied by x-ray absorption spectroscopy. <i>Science</i> , 2014, 346, 831-834.	12.6	391
2	Tailoring electrolyte solvation for Li metal batteries cycled at ultra-low temperature. <i>Nature Energy</i> , 2021, 6, 303-313.	39.5	386
3	Entropy and the driving force for the filling of carbon nanotubes with water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 11794-11798.	7.1	287
4	An All-Fluorinated Ester Electrolyte for Stable High-Voltage Li Metal Batteries Capable of Ultra-Low-Temperature Operation. <i>ACS Energy Letters</i> , 2020, 5, 1438-1447.	17.4	214
5	Polysulfide-Blocking Microporous Polymer Membrane Tailored for Hybrid Li-Sulfur Flow Batteries. <i>Nano Letters</i> , 2015, 15, 5724-5729.	9.1	153
6	Thermodynamics of liquids: standard molar entropies and heat capacities of common solvents from 2PT molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 169-181.	2.8	144
7	X-ray Absorption Spectra of Dissolved Polysulfides in Lithium-Sulfur Batteries from First-Principles. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1547-1551.	4.6	134
8	Molecular understanding of polyelectrolyte binders that actively regulate ion transport in sulfur cathodes. <i>Nature Communications</i> , 2017, 8, 2277.	12.8	117
9	Characterization of Polysulfide Radicals Present in an Ether-Based Electrolyte of a Lithium-Sulfur Battery During Initial Discharge Using In Situ X-ray Absorption Spectroscopy Experiments and First-Principles Calculations. <i>Advanced Energy Materials</i> , 2015, 5, 1500285.	19.5	107
10	Electrolyte design implications of ion-pairing in low-temperature Li metal batteries. <i>Energy and Environmental Science</i> , 2022, 15, 1647-1658.	30.8	89
11	Fingerprinting Lithium-Sulfur Battery Reaction Products by X-ray Absorption Spectroscopy. <i>Journal of the Electrochemical Society</i> , 2014, 161, A1100-A1106.	2.9	76
12	On the absolute thermodynamics of water from computer simulations: A comparison of first-principles molecular dynamics, reactive and empirical force fields. <i>Journal of Chemical Physics</i> , 2012, 137, 244507.	3.0	59
13	Universal Relationship between Molecular Structure and Crystal Structure in Peptoid Polymers and Prevalence of the <i>cis</i> Backbone Conformation. <i>Journal of the American Chemical Society</i> , 2018, 140, 827-833.	13.7	52
14	Ultrahigh coulombic efficiency electrolyte enables Li SPAN batteries with superior cycling performance. <i>Materials Today</i> , 2021, 42, 17-28.	14.2	50
15	Hydrophobic Segregation, Phase Transitions and the Anomalous Thermodynamics of Water/Methanol Mixtures. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13905-13912.	2.6	46
16	Absolute Entropy and Energy of Carbon Dioxide Using the Two-Phase Thermodynamic Model. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1893-1901.	5.3	44
17	X-ray spectroscopy as a probe for lithium polysulfide radicals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7743-7753.	2.8	43
18	Sub-nanometer confinement enables facile condensation of gas electrolyte for low-temperature batteries. <i>Nature Communications</i> , 2021, 12, 3395.	12.8	42

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19	Thermodynamic origins of the solvent-dependent stability of lithium polysulfides from first principles. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1441-1448.	2.8	41
20	The Role of Confined Water in Ionic Liquid Electrolytes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 556-559.	4.6	36
21	Arginine, a Key Residue for the Enhancing Ability of an Antifreeze Protein of the Beetle <i>Dendroides canadensis</i> . <i>Biochemistry</i> , 2009, 48, 9696-9703.	2.5	35
22	Multilayer Two-Dimensional Water Structure Confined in MoS ₂ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 16021-16028.	3.1	35
23	Interfacial Thermodynamics of Water and Six Other Liquid Solvents. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5943-5956.	2.6	32
24	Molecular-Scale Structure of Electrode-Electrolyte Interfaces: The Case of Platinum in Aqueous Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2018, 140, 16237-16244.	13.7	32
25	Experimental Validation of the Predicted Binding Site of Escherichia coli K1 Outer Membrane Protein A to Human Brain Microvascular Endothelial Cells. <i>Journal of Biological Chemistry</i> , 2010, 285, 37753-37761.	3.4	30
26	Stereoselective Growth of Small Molecule Patches on Nanoparticles. <i>Journal of the American Chemical Society</i> , 2021, 143, 12138-12144.	13.7	30
27	Nuclear Quantum Effects in Hydrophobic Nanoconfinement. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5530-5535.	4.6	26
28	Table-top extreme ultraviolet second harmonic generation. <i>Science Advances</i> , 2021, 7, .	10.3	26
29	pH-Dependent Conformations for Hyperbranched Poly(ethylenimine) from All-Atom Molecular Dynamics. <i>Macromolecules</i> , 2018, 51, 2187-2194.	4.8	20
30	Rate Constants of Electrochemical Reactions in a Lithium-Sulfur Cell Determined by Operando X-ray Absorption Spectroscopy. <i>Journal of the Electrochemical Society</i> , 2018, 165, A3487-A3495.	2.9	20
31	Quantum mechanics based force field for carbon (QMFF-Cx) validated to reproduce the mechanical and thermodynamics properties of graphite. <i>Journal of Chemical Physics</i> , 2010, 133, 134114.	3.0	18
32	A low-cost sulfate-based all iron redox flow battery. <i>Journal of Power Sources</i> , 2021, 513, 230457.	7.8	18
33	Role of Specific Cations and Water Entropy on the Stability of Branched DNA Motif Structures. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12159-12167.	2.6	17
34	Extreme Ultraviolet Second Harmonic Generation Spectroscopy in a Polar Metal. <i>Nano Letters</i> , 2021, 21, 6095-6101.	9.1	17
35	Solvent selection criteria for temperature-resilient lithium-sulfur batteries. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	17
36	Liquid Sulfur Impregnation of Microporous Carbon Accelerated by Nanoscale Interfacial Effects. <i>Nano Letters</i> , 2017, 17, 2517-2523.	9.1	16

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37	Polarization-Resolved Extreme-Ultraviolet Second-Harmonic Generation from LiNbO_3 . Physical Review Letters, 2021, 127, 237402.	7.8	15
38	Oxidative Stabilization of Dilute Ether Electrolytes via Anion Modification. ACS Energy Letters, 2022, 7, 675-682.	17.4	15
39	Angstrom-Resolved Interfacial Structure in Buried Organic-Inorganic Junctions. Physical Review Letters, 2021, 127, 096801.	7.8	14
40	Ferroelectric Modulation of Surface Electronic States in BaTiO_3 for Enhanced Hydrogen Evolution Activity. Nano Letters, 2022, 22, 4276-4284.	9.1	13
41	Predicting the Ion Desolvation Pathway of Lithium Electrolytes and Their Dependence on Chemistry and Temperature. Journal of Physical Chemistry Letters, 2022, 13, 4426-4433.	4.6	12
42	The purported square ice in bilayer graphene is a nanoscale, monolayer object. Journal of Chemical Physics, 2019, 150, 231101.	3.0	7
43	Dimensionality dependence of the Kauzmann temperature: A case study using bulk and confined water. Journal of Chemical Physics, 2021, 154, 164510.	3.0	5
44	Entropic Stabilization of Water at Graphitic Interfaces. Journal of Physical Chemistry Letters, 2021, 12, 9162-9168.	4.6	5
45	Complete inhibition of a polyol nucleation by a micromolar biopolymer additive. Cell Reports Physical Science, 2022, 3, 100723.	5.6	3
46	The phase diagram of carbon dioxide from correlation functions and a many-body potential. Journal of Chemical Physics, 2021, 155, 024503.	3.0	0