Chao Zhang

List of Publications by Year
in descending order

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Version: 2024-02-01

41 papers	1,292 citations	304743 22 h-index	361022 35 g-index
46 all docs	46 docs citations	46 times ranked	1503 citing authors

#	Article	IF	Citations
1	Artificial Intelligence Applied to Battery Research: Hype or Reality?. Chemical Reviews, 2022, 122, 10899-10969.	47.7	153
2	Finite-field coupling via learning the charge response kernel. Electronic Structure, 2022, 4, 014012.	2.8	6
3	Transference Number in Polymer Electrolytes: Mind the Reference-Frame Gap. Journal of the American Chemical Society, 2022, 144, 7583-7587.	13.7	39
4	Lithium electrodeposition for energy storage: filling the gap between theory and experiment. Materials Today Energy, 2022, 28, 101060.	4.7	3
5	Modelling Bulk Electrolytes and Electrolyte Interfaces with Atomistic Machine Learning. Batteries and Supercaps, 2021, 4, 585-595.	4.7	29
6	Origin of Asymmetric Electric Double Layers at Electrified Oxide/Electrolyte Interfaces. Journal of Physical Chemistry Letters, 2021, 12, 4616-4622.	4.6	15
7	Machine learning inference of molecular dipole moment in liquid water. Machine Learning: Science and Technology, 2021, 2, 03LT03.	5.0	4
8	Importance of the Ion-Pair Lifetime in Polymer Electrolytes. Journal of Physical Chemistry Letters, 2021, 12, 8460-8464.	4.6	15
9	Training algorithm matters for the performance of neural network potential: A case study of Adam and the Kalman filter optimizers. Journal of Chemical Physics, 2021, 155, 204108.	3.0	5
10	Temperature effects on the ionic conductivity in concentrated alkaline electrolyte solutions. Physical Chemistry Chemical Physics, 2020, 22, 10426-10430.	2.8	25
11	Computing Surface Acidity Constants of Proton Hopping Groups from Density Functional Theory-Based Molecular Dynamics: Application to the SnO₂(110)/H₂O Interface. Journal of Chemical Theory and Computation, 2020, 16, 6520-6527.	5.3	16
12	Effects of Solvent Polarity on Li-ion Diffusion in Polymer Electrolytes: An All-Atom Molecular Dynamics Study with Charge Scaling. Journal of Physical Chemistry B, 2020, 124, 8124-8131.	2.6	35
13	Role of Viscosity in Deviations from the Nernstâ€“Einstein Relation. Journal of Physical Chemistry B, 2020, 124, 4774-4780.	2.6	22
14	Electronic conductivity of polymer electrolytes: electronic charge transport properties of LiTFSI-doped PEO. Physical Chemistry Chemical Physics, 2020, 22, 7680-7684.	2.8	24
15	Electromechanics of the liquid water vapour interface. Physical Chemistry Chemical Physics, 2020, 22, 10676-10686.	2.8	14
16	PiNN: A Python Library for Building Atomic Neural Networks of Molecules and Materials. Journal of Chemical Information and Modeling, 2020, 60, 1184-1193.	5.4	48
17	Modelling electrochemical systems with finite field molecular dynamics. JPhys Energy, 2020, 2, 032005.	5.3	38
18	Coupling of Surface Chemistry and Electric Double Layer at TiO₂ Electrochemical Interfaces. Journal of Physical Chemistry Letters, 2019, 10, 3871-3876.	4.6	53

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19	Experimental and molecular dynamics study of the ionic conductivity in aqueous LiCl electrolytes. Chemical Physics Letters, 2019, 729, 6-10.	2.6	14
20	Finite electric displacement simulations of polar ionic solid-electrolyte interfaces: Application to NaCl(111)/aqueous NaCl solution. Journal of Chemical Physics, 2019, 150, 041716.	3.0	19
21	Note: On the dielectric constant of nanoconfined water. Journal of Chemical Physics, 2018, 148, 156101.	3.0	41
22	Conducting Polymer Paper-Derived Mesoporous 3D N-doped Carbon Current Collectors for Na and Li Metal Anodes: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2018, 122, 23352-23363.	3.1	27
23	Communication: Computing the Helmholtz capacitance of charged insulator-electrolyte interfaces from the supercell polarization. Journal of Chemical Physics, 2018, 149, 031103.	3.0	11
24	Interfacial water molecules at biological membranes: Structural features and role for lateral proton diffusion. PLoS ONE, 2018, 13, e0193454.	2.5	12
25	Charge compensation at the interface between the polar NaCl(111) surface and a NaCl aqueous solution. Journal of Chemical Physics, 2017, 147, 104702.	3.0	15
26	Origin of proton affinity to membrane/water interfaces. Scientific Reports, 2017, 7, 4553.	3.3	49
27	Computing the Kirkwood g-Factor by Combining Constant Maxwell Electric Field and Electric Displacement Simulations: Application to the Dielectric Constant of Liquid Water. Journal of Physical Chemistry Letters, 2016, 7, 2696-2701.	4.6	63
28	Finite field methods for the supercell modeling of charged insulator/electrolyte interfaces. Physical Review B, 2016, 94, .	3.2	42
29	Computing the dielectric constant of liquid water at constant dielectric displacement. Physical Review B, 2016, 93, .	3.2	49
30	Competing factors on the frequency separation between the OH stretching modes in water. Journal of Molecular Liquids, 2015, 205, 42-45.	4.9	13
31	Study of water adsorption and capillary bridge formation for SiO₂nanoparticle layers by means of a combined in situ FT-IR reflection spectroscopy and QCM-D set-up. Physical Chemistry Chemical Physics, 2014, 16, 7377-7384.	2.8	39
32	Asymmetric Environmental Effects on the Structure and Vibrations ofcis-[Pt(NH3)2Cl2] in Condensed Phases. Journal of Physical Chemistry B, 2014, 118, 11487-11495.	2.6	9
33	Vibrational Signature of Water Molecules in Asymmetric Hydrogen Bonding Environments. Journal of Physical Chemistry Letters, 2013, 4, 3245-3250.	4.6	46
34	Role of the Membrane Dipole Potential for Proton Transport in Gramicidin A Embedded in a DMPC Bilayer. Journal of Chemical Theory and Computation, 2013, 9, 3826-3831.	5.3	17
35	Reply to â€œComment on `Structure and dynamics of liquid water on rutile TiO2(110)'â€‰â€• Physical Review B, 2012, 85, .	3.2	30
36	Salt effects on water/hydrophobic liquid interfaces: a molecular dynamics study. Journal of Physics Condensed Matter, 2012, 24, 124109.	1.8	19

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37	Water at hydrophobic interfaces delays proton surface-to-bulk transfer and provides a pathway for lateral proton diffusion. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9744-9749.	7.1	104
38	Molecular Dynamics in Physiological Solutions: Force Fields, Alkali Metal Ions, and Ionic Strength. Journal of Chemical Theory and Computation, 2010, 6, 2167-2175.	5.3	56
39	Isothermal section of the Cuâ€“Mnâ€“Si ternary system at 700 Â°C. Journal of Alloys and Compounds, 2010, 492, 190-195.	5.5	9
40	Thermodynamic modeling of the Vâ€“Si system supported by key experiments. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 320-325.	1.6	40
41	An investigation on the thermodynamic stability of V6Si5. Journal of Materials Science, 2007, 42, 7046-7048.	3.7	23