Chenghan Li

List of Publications by Year
in descending order

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20 papers	387 citations	933447 10 h-index	839539 18 g-index
22 all docs	22 docs citations	22 times ranked	360 citing authors

#	Article	IF	Citations
1	Key Factors Governing Initial Stages of Lipid Droplet Formation. Journal of Physical Chemistry B, 2022, 126, 453-462.	2.6	15
2	Using Machine Learning to Greatly Accelerate Path Integral Ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 599-604.	5.3	11
3	Static and Dynamic Correlations in Water: Comparison of Classical Ab Initio Molecular Dynamics at Elevated Temperature with Path Integral Simulations at Ambient Temperature. Journal of Chemical Theory and Computation, 2022, 18, 2124-2131.	5.3	16
4	Using Hyperoptimized Tensor Networks and First-Principles Electronic Structure to Simulate the Experimental Properties of the Giant {Mn₈₄} Torus. Journal of Physical Chemistry Letters, 2022, 13, 2365-2370.	4.6	3
5	Proton coupling and the multiscale kinetic mechanism of a peptide transporter. Biophysical Journal, 2022, 121, 2266-2278.	0.5	9
6	The hopping mechanism of the hydrated excess proton and its contribution to proton diffusion in water. Journal of Chemical Physics, 2021, 154, 194506.	3.0	12
7	Key computational findings reveal proton transfer as driving the functional cycle in the phosphate transporter PiPT. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	10
8	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. Journal of the American Chemical Society, 2021, 143, 10203-10213.	13.7	35
9	Toward a Multipathway Perspective: pH-Dependent Kinetic Selection of Competing Pathways and the Role of the Internal Glutamate in Cl^{â€“}/H⁺ Antiporters. Journal of Physical Chemistry B, 2021, 125, 7975-7984.	2.6	6
10	Using Constrained Density Functional Theory to Track Proton Transfers and to Sample Their Associated Free Energy Surface. Journal of Chemical Theory and Computation, 2021, 17, 5759-5765.	5.3	9
11	Accurate and Transferable Reactive Molecular Dynamics Models from Constrained Density Functional Theory. Journal of Physical Chemistry B, 2021, 125, 10471-10480.	2.6	11
12	Resolving the Structural Debate for the Hydrated Excess Proton in Water. Journal of the American Chemical Society, 2021, 143, 18672-18683.	13.7	31
13	A quantitative paradigm for water-assisted proton transport through proteins and other confined spaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	16
14	Molecular Origins of the Barriers to Proton Transport in Acidic Aqueous Solutions. Journal of Physical Chemistry B, 2020, 124, 8868-8876.	2.6	12
15	Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale. Biophysical Journal, 2020, 119, 1033-1040.	0.5	11
16	What Coordinate Best Describes the Affinity of the Hydrated Excess Proton for the Airâ€“Water Interface?. Journal of Physical Chemistry B, 2020, 124, 5039-5046.	2.6	9
17	Understanding and Tracking the Excess Proton in Ab Initio Simulations; Insights from IR Spectra. Journal of Physical Chemistry B, 2020, 124, 5696-5708.	2.6	22
18	Water-Assisted Proton Transport in Confined Nanochannels. Journal of Physical Chemistry C, 2020, 124, 16186-16201.	3.1	12

#	Article	IF	Citations
19	Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules. Journal of the American Chemical Society, 2019, 141, 13421-13433.	13.7	56
20	Proton movement and coupling in the POT family of peptide transporters. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13182-13187.	7.1	81