

Chenghan Li

List of Publications by Year in descending order

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Version: 2024-02-01

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	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
2	Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules. Journal of the American Chemical Society, 2019, 141, 13421-13433.	13.7	56
3	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. Journal of the American Chemical Society, 2021, 143, 10203-10213.	13.7	35
4	Resolving the Structural Debate for the Hydrated Excess Proton in Water. Journal of the American Chemical Society, 2021, 143, 18672-18683.	13.7	31
5	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
6	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
7	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
8	Key Factors Governing Initial Stages of Lipid Droplet Formation. Journal of Physical Chemistry B, 2022, 126, 453-462.	2.6	15
9	Molecular Origins of the Barriers to Proton Transport in Acidic Aqueous Solutions. Journal of Physical Chemistry B, 2020, 124, 8868-8876.	2.6	12
10	Water-Assisted Proton Transport in Confined Nanochannels. Journal of Physical Chemistry C, 2020, 124, 16186-16201.	3.1	12
11	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
12	Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale. Biophysical Journal, 2020, 119, 1033-1040.	0.5	11
13	Accurate and Transferable Reactive Molecular Dynamics Models from Constrained Density Functional Theory. Journal of Physical Chemistry B, 2021, 125, 10471-10480.	2.6	11
14	Using Machine Learning to Greatly Accelerate Path Integral <i>Ab Initio</i> Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 599-604.	5.3	11
15	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
16	What Coordinate Best Describes the Affinity of the Hydrated Excess Proton for the Air–Water Interface?. Journal of Physical Chemistry B, 2020, 124, 5039-5046.	2.6	9
17	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
18	Proton coupling and the multiscale kinetic mechanism of a peptide transporter. Biophysical Journal, 2022, 121, 2266-2278.	0.5	9

#	ARTICLE	IF	CITATIONS
19	Toward a Multipathway Perspective: pH-Dependent Kinetic Selection of Competing Pathways and the Role of the Internal Glutamate in Cl ⁻ /H ⁺ Antiporters. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7975-7984.	2.6	6
20	Using Hyperoptimized Tensor Networks and First-Principles Electronic Structure to Simulate the Experimental Properties of the Giant {Mn ₈₄ } Torus. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2365-2370.	4.6	3