C Mark Maupin

List of Publications by Year
in descending order

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37 papers	1,421 citations	331670 21 h-index	330143 37 g-index
37 all docs	37 docs citations	37 times ranked	1732 citing authors

#	Article	IF	Citations
1	Proton Solvation and Transport in Aqueous and Biomolecular Systems:Â Insights from Computer Simulations. Journal of Physical Chemistry B, 2007, 111, 4300-4314.	2.6	279
2	Atomic Crystal and Molecular Dynamics Simulation Structures of Human Carbonic Anhydrase II:Â Insights into the Proton Transfer Mechanismâ€,â€¡. Biochemistry, 2007, 46, 2930-2937.	2.5	155
3	Elucidation of the Proton Transport Mechanism in Human Carbonic Anhydrase II. Journal of the American Chemical Society, 2009, 131, 7598-7608.	13.7	84
4	The Self-Consistent Charge Density Functional Tight Binding Method Applied to Liquid Water and the Hydrated Excess Proton: Benchmark Simulations. Journal of Physical Chemistry B, 2010, 114, 6922-6931.	2.6	67
5	Anion exchange membranes composed of a poly(2,6-dimethyl-1,4-phenylene oxide) random copolymer functionalized with a bulky phosphonium cation. Journal of Membrane Science, 2016, 506, 50-59.	8.2	67
6	A Multistate Empirical Valence Bond Description of Protonatable Amino Acidsâ€. Journal of Physical Chemistry A, 2006, 110, 631-639.	2.5	62
7	Preferred Orientations of His64 in Human Carbonic Anhydrase IIâ€. Biochemistry, 2007, 46, 2938-2947.	2.5	60
8	Chemical Rescue of Enzymes: Proton Transfer in Mutants of Human Carbonic Anhydrase II. Journal of the American Chemical Society, 2011, 133, 6223-6234.	13.7	56
9	Application of the SCC-DFTB Method to Hydroxide Water Clusters and Aqueous Hydroxide Solutions. Journal of Physical Chemistry B, 2013, 117, 5165-5179.	2.6	56
10	Defining Condensed Phase Reactive Force Fields from ab Initio Molecular Dynamics Simulations: The Case of the Hydrated Excess Proton. Journal of Chemical Theory and Computation, 2010, 6, 3223-3232.	5.3	38
11	Origins of Enhanced Proton Transport in the Y7F Mutant of Human Carbonic Anhydrase II. Journal of the American Chemical Society, 2008, 130, 11399-11408.	13.7	35
12	Electronic Structure and Spectroscopic Analysis of 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide Ion Pair. Journal of Physical Chemistry A, 2014, 118, 6873-6882.	2.5	35
13	Transport and Morphology of a Proton Exchange Membrane Based on a Doubly Functionalized Perfluorosulfonic Imide Side Chain Perflourinated Polymer. Chemistry of Materials, 2020, 32, 38-59.	6.7	33
14	Proton transport in carbonic anhydrase: Insights from molecular simulation. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2010, 1804, 332-341.	2.3	31
15	Structural insight into activity enhancement and inhibition of H64A carbonic anhydrase II by imidazoles. IUCrJ, 2014, 1, 129-135.	2.2	31
16	Insights into the Glycyl Radical Enzyme Active Site of Benzylsuccinate Synthase: A Computational Study. Journal of the American Chemical Society, 2013, 135, 12279-12288.	13.7	30
17	Coupling Protein Dynamics with Proton Transport in Human Carbonic Anhydrase II. Journal of Physical Chemistry B, 2016, 120, 8389-8404.	2.6	27
18	A Combined Theoretical and Experimental Investigation of the Transport Properties of Water in a Perfluorosulfonic Acid Proton Exchange Membrane Doped with the Heteropoly Acids, H₃PW₁₂O₄₀ or H₄SiW₁₂O₄₀. Journal of Physical Chemistry C, 2014, 118, 854-863.	3.1	26

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19	A Novel Optical Diagnostic for In Situ Measurements of Lithium Polysulfides in Battery Electrolytes. Applied Spectroscopy, 2017, 71, 1593-1599.	2.2	26
20	Impact of Water-Dilution on the Solvation Properties of the Ionic Liquid 1-Methyltriethoxy-3-ethylimidazolium Acetate for Model Biomass Molecules. Journal of Physical Chemistry B, 2017, 121, 843-853.	2.6	23
21	Enhancing Proton Transport and Membrane Lifetimes in Perfluorosulfonic Acid Proton Exchange Membranes: A Combined Computational and Experimental Evaluation of the Structure and Morphology Changes Due to H₃PW₁₂O₄₀ Doping. Journal of Physical Chemistry C, 2014, 118, 20193-20202.	3.1	21
22	Elucidating the conformational energetics of glucose and cellobiose in ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 10668-10678.	2.8	19
23	In silico insights into the solvation characteristics of the ionic liquid 1-methyltriethoxy-3-ethylimidazolium acetate for cellulosic biomass. Physical Chemistry Chemical Physics, 2016, 18, 23715-23726.	2.8	17
24	pKa Determination of Histidine Residues in Î±-Conotoxin MII Peptides by 1H NMR and Constant pH Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2013, 117, 2653-2661.	2.6	14
25	Acetylcholine Promotes Binding of Î±â€Conotoxin MII at Î±₃Î²₂ Nicotinic Acetylcholine Receptors. ChemBioChem, 2014, 15, 413-424.	2.6	14
26	Molecular Simulations of Fattyâ€Acid Methyl Esters and Representative Biodiesel Mixtures. ChemPhysChem, 2015, 16, 2810-2817.	2.1	14
27	Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism â€“ a gas-phaseab initiostudy. Physical Chemistry Chemical Physics, 2015, 17, 4054-4066.	2.8	14
28	Impact of water dilution and cation tail length on ionic liquid characteristics: Interplay between polar and non-polar interactions. Journal of Chemical Physics, 2016, 145, 064504.	3.0	14
29	Effect of Active-site Mutation at Asn67 on the Proton Transfer Mechanism of Human Carbonic Anhydrase II. Biochemistry, 2009, 48, 7996-8005.	2.5	13
30	Solvation Dynamics of HEHEHP Ligand at the Liquidâ€“Liquid Interface. Journal of Physical Chemistry B, 2018, 122, 5999-6006.	2.6	12
31	Computational Evaluation of the Dynamic Fluctuations of Peripheral Loops Enclosing the Catalytic Tunnel of a Family 7 Cellobiohydrolase. Journal of Physical Chemistry B, 2014, 118, 5340-5349.	2.6	8
32	Computational Evaluations of Charge Coupling and Hydrogen Bonding in the Active Site of a Family 7 Cellobiohydrolase. Journal of Physical Chemistry B, 2014, 118, 434-448.	2.6	8
33	Optical measurements of impurities in room-temperature ionic liquids. Journal of Quantitative Spectroscopy and Radiative Transfer, 2014, 133, 300-310.	2.3	8
34	Random and Block Sulfonated Polyaramides as Advanced Proton Exchange Membranes. Journal of Physical Chemistry C, 2015, 119, 24724-24732.	3.1	8
35	Identifying the Enzymatic Mode of Action for Cellulase Enzymes by Means of Docking Calculations and a Machine Learning Algorithm. AIMS Molecular Science, 2014, 1, 59-80.	0.5	6
36	The impact of active site protonation on substrate ring conformation in Melanocarpus albomyces cellobiohydrolase Cel7B. Physical Chemistry Chemical Physics, 2015, 17, 16947-16958.	2.8	5

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37	A charge-modified general amber force field for phospholipids: improved structural properties in the tensionless ensemble. Molecular Simulation, 2015, 41, 1449-1458.	2.0	5