Martin Brehm

List of Publications by Year
in descending order

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52 papers	3,797 citations	218381 26 h-index	174990 52 g-index
55 all docs	55 docs citations	55 times ranked	3328 citing authors

#	Article	IF	Citations
1	Raman Optical Activity of Nâ€Acetylâ€Lâ€Cysteine in Water and in Methanol: The â€œClustersâ€inâ€aâ€Liquidâ€•Model and ab Initio Molecular Dynamics Simulations. ChemPhysChem, 2022, 23, .	1.0	8
2	A force field for bio-polymers in ionic liquids (BILFF) â€“ part 1: [EMIm][OAc]/water mixtures. Physical Chemistry Chemical Physics, 2021, 23, 1242-1253.	1.3	8
3	Switching between Proton Vacancy and Excess Proton Transfer Pathways in the Reaction between 7-Hydroxyquinoline and Formate. Journal of Physical Chemistry A, 2021, 125, 1845-1859.	1.1	10
4	Optimized Atomic Partial Charges and Radii Defined by Radical Voronoi Tessellation of Bulk Phase Simulations. Molecules, 2021, 26, 1875.	1.7	4
5	Unraveling Local Structure of Molten Salts via X-ray Scattering, Raman Spectroscopy, and Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 5971-5982.	1.2	23
6	Liquid structure and dynamics in the choline acetate:urea 1:2 deep eutectic solvent. Journal of Chemical Physics, 2021, 154, 244501.	1.2	17
7	Liquid structure of a choline chloride-water natural deep eutectic solvent: A molecular dynamics characterization. Journal of Molecular Liquids, 2021, 331, 115750.	2.3	37
8	Efficient EOM-CC-based Protocol for the Calculation of Electron Affinity of Solvated Nucleobases: Uracil as a Case Study. Journal of Chemical Theory and Computation, 2021, 17, 105-116.	2.3	16
9	Dissolving Cellulose in 1,2,3-Triazolium- and Imidazolium-Based Ionic Liquids with Aromatic Anions. Molecules, 2020, 25, 3539.	1.7	23
10	Characterization of Aqueous Lower-Polarity Solvation Shells Around Amphiphilic 2,2,6,6-Tetramethylpiperidine-1-oxyl Radicals in Water. Journal of Physical Chemistry B, 2020, 124, 8601-8609.	1.2	14
11	Exploring Free Energy Profiles of Enantioselective Organocatalytic Aldol Reactions under Full Solvent Influence. Molecules, 2020, 25, 5861.	1.7	7
12	Dynamical matrix propagator scheme for large-scale proton dynamics simulations. Journal of Chemical Physics, 2020, 152, 114114.	1.2	6
13	Exploring non-equilibrium molecular dynamics of mobile protons in the solid acid CsH2PO4 at the micrometer and microsecond scale. Journal of Chemical Physics, 2020, 152, 164110.	1.2	5
14	TRAVISâ€”A free analyzer for trajectories from molecular simulation. Journal of Chemical Physics, 2020, 152, 164105.	1.2	342
15	From flat to tilted: gradual interfaces in organic thin film growth. Nanoscale, 2020, 12, 3834-3845.	2.8	4
16	Computing Bulk Phase Resonance Raman Spectra from ab Initio Molecular Dynamics and Real-Time TDDFT. Journal of Chemical Theory and Computation, 2019, 15, 3901-3905.	2.3	14
17	Triazolium-Based Ionic Liquids: A Novel Class of Cellulose Solvents. Journal of Physical Chemistry B, 2019, 123, 3994-4003.	1.2	43
18	Simulating structure and dynamics in small droplets of 1-ethyl-3-methylimidazolium acetate. Journal of Chemical Physics, 2018, 148, 193802.	1.2	19

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19	Structure and lifetimes in ionic liquids and their mixtures. Faraday Discussions, 2018, 206, 219-245.	1.6	74
20	Nanoscopic structures and molecular interactions leading to a dystectic and two eutectic points in [EMIm][Cl]/urea mixtures. Physical Chemistry Chemical Physics, 2018, 20, 29591-29600.	1.3	14
21	An Efficient Lossless Compression Algorithm for Trajectories of Atom Positions and Volumetric Data. Journal of Chemical Information and Modeling, 2018, 58, 2092-2107.	2.5	14
22	Salt Bridge in Aqueous Solution: Strong Structural Motifs but Weak Enthalpic Effect. Scientific Reports, 2018, 8, 13626.	1.6	41
23	Glutathione Adduct Patterns of Michael-Acceptor Carbonyls. Environmental Science & Technology, 2017, 51, 4018-4026.	4.6	13
24	An Integrated Data-Driven Strategy for Safe-by-Design Nanoparticles: The FP7 MODERN Project. Advances in Experimental Medicine and Biology, 2017, 947, 257-301.	0.8	6
25	Influence of Small Fluorophilic and Lipophilic Organic Molecules on Dipalmitoylphosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2017, 121, 8311-8321.	1.2	5
26	Computing Bulk Phase Raman Optical Activity Spectra from ab initio Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2017, 8, 3409-3414.	2.1	24
27	Polyphilic Interactions as Structural Driving Force Investigated by Molecular Dynamics Simulation (Project 7). Polymers, 2017, 9, 445.	2.0	1
28	Domain Analysis in Nanostructured Liquids: A Postâ€Molecular Dynamics Study at the Example of Ionic Liquids. ChemPhysChem, 2015, 16, 3271-3277.	1.0	103
29	Triphilic Ionicâ€Liquid Mixtures: Fluorinated and Nonâ€fluorinated Aprotic Ionicâ€Liquid Mixtures. ChemPhysChem, 2015, 16, 3325-3333.	1.0	107
30	Anaerobic Microbial Transformation of Halogenated Aromatics and Fate Prediction Using Electron Density Modeling. Environmental Science & Technology, 2015, 49, 6018-6028.	4.6	60
31	Voronoi dipole moments for the simulation of bulk phase vibrational spectra. Physical Chemistry Chemical Physics, 2015, 17, 3207-3213.	1.3	100
32	How Can a Carbene be Active in an Ionic Liquid?. Chemistry - A European Journal, 2014, 20, 1622-1629.	1.7	48
33	Understanding ionic liquids from theoretical methods. Journal of Molecular Liquids, 2014, 192, 71-76.	2.3	64
34	Simulating the vibrational spectra of ionic liquid systems: 1-Ethyl-3-methylimidazolium acetate and its mixtures. Journal of Chemical Physics, 2014, 141, 024510.	1.2	77
35	Interactions in ionic liquids probed by in situ NMR spectroscopy. Journal of Molecular Liquids, 2014, 192, 55-58.	2.3	37
36	Understanding the evaporation of ionic liquids using the example of 1-ethyl-3-methylimidazolium ethylsulfate. Physical Chemistry Chemical Physics, 2013, 15, 18424.	1.3	30

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37	A Theoretical and Experimental Chemistâ€™s Joint View on Hydrogen Bonding in Ionic Liquids and Their Binary Mixtures. Topics in Current Chemistry, 2013, 351, 149-187.	4.0	26
38	Computing vibrational spectra from ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 6608.	1.3	414
39	Carbene Formation in Ionic Liquids: Spontaneous, Induced, or Prohibited?. Journal of Physical Chemistry B, 2013, 117, 5898-5907.	1.2	109
40	Liquid Structure and Cluster Formation in Ionic Liquid/Water Mixtures â€“ An Extensive ab initio Molecular Dynamics Study on 1-Ethyl-3-Methylimidazolium Acetate/Water Mixtures â€“ Part. Zeitschrift Fur Physikalische Chemie, 2013, 227, 177-204.	1.4	48
41	A one-parameter quantum cluster equilibrium approach. Journal of Chemical Physics, 2012, 137, 164107.	1.2	11
42	On the ideality of binary mixtures of ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 13204.	1.3	90
43	Proton transfer and polarity changes in ionic liquidâ€“water mixtures: a perspective on hydrogen bonds from ab initio molecular dynamics at the example of 1-ethyl-3-methylimidazolium acetateâ€“water mixturesâ€”Part 1. Physical Chemistry Chemical Physics, 2012, 14, 5030.	1.3	144
44	Short Time Dynamics of Ionic Liquids in AIMD-Based Power Spectra. Journal of Chemical Theory and Computation, 2012, 8, 1570-1579.	2.3	70
45	Effect of Dispersion on the Structure and Dynamics of the Ionic Liquid 1â€Ethylâ€3â€methylimidazolium Thiocyanate. ChemPhysChem, 2012, 13, 1845-1853.	1.0	81
46	TRAVIS - a free analyzer and visualizer for Monte Carlo and molecular dynamics trajectories. Journal of Cheminformatics, 2012, 4, .	2.8	18
47	Singular Value Decomposition for Analyzing Temperature- and Pressure-Dependent Radial Distribution Functions: Decomposition into Grund RDFs (GRDFs). Journal of Chemical Theory and Computation, 2011, 7, 3035-3039.	2.3	2
48	Ab initio molecular dynamics simulations of a binary system of ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 13617.	1.3	69
49	How Hydrogen Bonds Influence the Mobility of Imidazolium-Based Ionic Liquids. A Combined Theoretical and Experimental Study of 1-n-Butyl-3-methylimidazolium Bromide. Journal of Physical Chemistry B, 2011, 115, 15280-15288.	1.2	118
50	Performance of Quantum Chemically Derived Charges and Persistence of Ion Cages in Ionic Liquids. A Molecular Dynamics Simulations Study of 1-n-Butyl-3-methylimidazolium Bromide. Journal of Physical Chemistry B, 2011, 115, 693-702.	1.2	137
51	TRAVIS - A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories. Journal of Chemical Information and Modeling, 2011, 51, 2007-2023.	2.5	930
52	Unexpected Hydrogen Bond Dynamics in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15129-15132.	1.2	112