Martin Brehm

List of Publications by Year
in descending order

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Version: 2024-02-01

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	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
2	Computing vibrational spectra from ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 6608.	1.3	414
3	TRAVISâ€"A free analyzer for trajectories from molecular simulation. Journal of Chemical Physics, 2020, 152, 164105.	1.2	342
4	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
5	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
6	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
7	Unexpected Hydrogen Bond Dynamics in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15129-15132.	1.2	112
8	Carbene Formation in Ionic Liquids: Spontaneous, Induced, or Prohibited?. Journal of Physical Chemistry B, 2013, 117, 5898-5907.	1.2	109
9	Triphilic Ionicâ€Liquid Mixtures: Fluorinated and Nonâ€fluorinated Aprotic Ionicâ€Liquid Mixtures. ChemPhysChem, 2015, 16, 3325-3333.	1.0	107
10	Domain Analysis in Nanostructured Liquids: A Postâ€Molecular Dynamics Study at the Example of Ionic Liquids. ChemPhysChem, 2015, 16, 3271-3277.	1.0	103
11	Voronoi dipole moments for the simulation of bulk phase vibrational spectra. Physical Chemistry Chemical Physics, 2015, 17, 3207-3213.	1.3	100
12	On the ideality of binary mixtures of ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 13204.	1.3	90
13	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
14	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
15	Structure and lifetimes in ionic liquids and their mixtures. Faraday Discussions, 2018, 206, 219-245.	1.6	74
16	Short Time Dynamics of Ionic Liquids in AIMD-Based Power Spectra. Journal of Chemical Theory and Computation, 2012, 8, 1570-1579.	2.3	70
17	Ab initio molecular dynamics simulations of a binary system of ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 13617.	1.3	69
18	Understanding ionic liquids from theoretical methods. Journal of Molecular Liquids, 2014, 192, 71-76.	2.3	64

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19	Anaerobic Microbial Transformation of Halogenated Aromatics and Fate Prediction Using Electron Density Modeling. Environmental Science & Technology, 2015, 49, 6018-6028.	4.6	60
20	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
21	How Can a Carbene be Active in an Ionic Liquid?. Chemistry - A European Journal, 2014, 20, 1622-1629.	1.7	48
22	Triazolium-Based Ionic Liquids: A Novel Class of Cellulose Solvents. Journal of Physical Chemistry B, 2019, 123, 3994-4003.	1.2	43
23	Salt Bridge in Aqueous Solution: Strong Structural Motifs but Weak Enthalpic Effect. Scientific Reports, 2018, 8, 13626.	1.6	41
24	Interactions in ionic liquids probed by in situ NMR spectroscopy. Journal of Molecular Liquids, 2014, 192, 55-58.	2.3	37
25	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
26	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
27	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
28	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
29	Dissolving Cellulose in 1,2,3-Triazolium- and Imidazolium-Based Ionic Liquids with Aromatic Anions. Molecules, 2020, 25, 3539.	1.7	23
30	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
31	Simulating structure and dynamics in small droplets of 1-ethyl-3-methylimidazolium acetate. Journal of Chemical Physics, 2018, 148, 193802.	1.2	19
32	TRAVIS - a free analyzer and visualizer for Monte Carlo and molecular dynamics trajectories. Journal of Cheminformatics, 2012, 4, .	2.8	18
33	Liquid structure and dynamics in the choline acetate:urea 1:2 deep eutectic solvent. Journal of Chemical Physics, 2021, 154, 244501.	1.2	17
34	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
35	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
36	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

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37	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
38	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
39	Glutathione Adduct Patterns of Michael-Acceptor Carbonyls. Environmental Science & Technology, 2017, 51, 4018-4026.	4.6	13
40	A one-parameter quantum cluster equilibrium approach. Journal of Chemical Physics, 2012, 137, 164107.	1.2	11
41	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
42	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
43	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
44	Exploring Free Energy Profiles of Enantioselective Organocatalytic Aldol Reactions under Full Solvent Influence. Molecules, 2020, 25, 5861.	1.7	7
45	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
46	Dynamical matrix propagator scheme for large-scale proton dynamics simulations. Journal of Chemical Physics, 2020, 152, 114114.	1.2	6
47	Influence of Small Fluorophilic and Lipophilic Organic Molecules on Dipalmitoylphosphatidylcholine Bilayers. Journal of Physical Chemistry B, 2017, 121, 8311-8321.	1.2	5
48	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
49	Optimized Atomic Partial Charges and Radii Defined by Radical Voronoi Tessellation of Bulk Phase Simulations. Molecules, 2021, 26, 1875.	1.7	4
50	From flat to tilted: gradual interfaces in organic thin film growth. Nanoscale, 2020, 12, 3834-3845.	2.8	4
51	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
52	Polyphilic Interactions as Structural Driving Force Investigated by Molecular Dynamics Simulation (Project 7). Polymers, 2017, 9, 445.	2.0	1