

49 Artikel in Zeitschriften mit „Peer Review“-Verfahren.

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- 49.) S. Roy, M. Brehm, S. Sharma, F. Wu, D. Maltsev, P. Halstenberg, L. Gallington, S. Mahurin, S. Dai, A. Ivanov, C. Margulis, V. Bryantsev: „Unraveling Local Structure of Molten Salts via X-Ray Scattering, Raman Spectroscopy, and ab initio Molecular Dynamics“, *J. Phys. Chem. B* **2021**, *accepted*.
- 48.) M. Brehm, M. Thomas: „Optimized Atomic Partial Charges and Radii Defined by Radical Voronoi Tessellation of Bulk Phase Simulations“, *Molecules* **2021**, *26 (7)*, 1875. (DOI 10.3390/molecules26071875 )
- 47.) M.-A. Codescu, M. Weiß, M. Brehm, O. Kornilov, D. Sebastiani, E. T. J. Nibbering: „Switching Between Proton Vacancy and Excess Proton Transfer Pathways in the Reaction Between 7-Hydroxyquinoline and Formate“, *J. Phys. Chem. A* **2021**, *125 (9)*, 1845–1859. (DOI 10.1021/acs.jpca.0c10191 )
- 46.) A. Triolo, F. Lo Celso, M. Brehm, V. Di Lisio, O. Russina: „Liquid Structure of a Choline Chloride-Water Natural Deep Eutectic Solvent: A Molecular Dynamics Characterization“, *J. Mol. Liq.* **2021**, *331*, 115750. (DOI 10.1016/j.molliq.2021.115750 )
- 45.) E. Roos, M. Brehm: „A Force Field for Bio-Polymers in Ionic Liquids (BILFF) – Part 1: [EMIm][OAc] / Water Mixtures“, *Phys. Chem. Chem. Phys.* **2021**, *23*, 1242–1253. (DOI 10.1039/D0CP04537C )
- 44.) M. Mukherjee, D. Tripathi, M. Brehm, C. Riplinger, A. K. Dutta: „Efficient EOM-CC-Based Protocol for the Calculation of Electron Affinity of Solvated Nucleobases: Uracil as a Case Study“, *J. Chem. Theory Comput.* **2021**, *17 (1)*, 105–116. (DOI 10.1021/acs.jctc.0c00655 )
- 43.) M. Weiß, M. Brehm: „Exploring Free Energy Profiles of Enantioselective Organocatalytic Aldol Reactions under Full Solvent Influence“, *Molecules* **2020**, *25 (24)*, 5861. (DOI 10.3390/molecules25245861 )
- 42.) J. Hunold, J. Eisermann, M. Brehm, D. Hinderberger: „Characterization of Aqueous Lower Polarity Solvation Shells Around Amphiphilic TEMPO Radicals in Water“, *J. Phys. Chem. B* **2020**, *124 (39)*, 8601–8609. (DOI 10.1021/acs.jpcc.0c04863 )
- 41.) M. Brehm, J. Radicke, M. Pulst, F. Shaabani, D. Sebastiani, J. Kressler: „Dissolving Cellulose in 1,2,3-Triazolium- and Imidazolium-Based Ionic Liquids with Aromatic Anions“, *Molecules* **2020**, *25*, 3539. (DOI 10.3390/molecules25153539 )
- 40.) M. Brehm, M. Thomas, S. Gehrke, B. Kirchner: „TRAVIS – A Free Analyzer for Trajectories from Molecular Simulation“, *J. Chem. Phys.* **2020**, *152 (16)*, 164105. (DOI 10.1063/5.0005078 )
- 39.) C. Dreßler, G. Kabbe, M. Brehm, D. Sebastiani: „Exploring Non-Equilibrium Molecular Dynamics of Mobile Protons in the Solid Acid CsH<sub>2</sub>PO<sub>4</sub> on the Micrometer and Microsecond Scale“, *J. Chem. Phys.* **2020**, *152 (16)*, 164110. (DOI 10.1063/5.0002167 )
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- 22.) M. Brehm, H. Weber, M. Thomas, O. Hollóczki, B. Kirchner: „Domain Analysis in Nanostructured Liquids: A Post-Molecular Dynamics Study at the Example of Ionic Liquids“, *ChemPhysChem* **2015**, *16* (15), 3271–3277. (DOI 10.1002/cphc.201500471)
- 21.) O. Hollóczki, M. Macchiagodena, H. Weber, M. Thomas, M. Brehm, A. Stark, O. Russina, A. Triolo, B. Kirchner: „Triphilic Ionic Liquid Mixtures: Fluorinated and Non-fluorinated Aprotic Ionic Liquid Mixtures“, *ChemPhysChem* **2015**, *16* (15), 3325–3333. (DOI 10.1002/cphc.201500473)
- 20.) A. Stark, M. Brehm, M. Brüssel, S. B. C. Lehmann, A. S. Pensado, M. Schöppke, B. Kirchner: „A Theoretical and Experimental Chemist’s Joint View on Hydrogen Bonding in Ionic Liquids and Their Binary Mixtures“, *Top. Curr. Chem.* **2014**, *351*, 149–187. (DOI 10.1007/128\_2013\_485)
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- 17.) S. Zahn, M. Brehm, M. Brüssel, O. Hollóczki, M. Kohagen, S. B. C. Lehmann, F. Malberg, A. S. Pensado, M. Schöppke, H. Weber, B. Kirchner: „Understanding Ionic Liquids from Theoretical Methods“, *J. Mol. Liq.* **2014**, *192*, 71–76. (DOI 10.1016/j.molliq.2013.08.015)
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