Modeling Liquid Phase Vibrational Spectra: From Molecular to Ionic Liquids

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Abstract:

We will present our recent developments for the calculation of infrared, [1] Raman, [1] and vibrational circular dichroism [2,3] spectra of flexible molecules in non-idle environments. [4] The calculation of such spectra requires: 1) a realistic description of the non-idle environment and 2) a sufficient sampling of the solvation shells and molecular conformations. We will show how these critical issues can be addressed to obtain robust predictions of liquid phase spectra. We further present applications of our methods to study chiral phenomena, e.g. asymmetrization and chirality transfer in (ionic) liquids, which can be used to develop new chiral selectors and separation processes. [5,6]

References:

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Biography:

Jan Blasius is a Ph.D. student in the research group of Prof. Barbara Kirchner. He studied chemistry at the Rheinische Friedrich-Wilhelms University of Bonn and obtained his B.Sc. (2017) and M.Sc. degrees (2019) after work in the group of Barbara Kirchner. In his B.Sc. thesis he investigated a new theoretical approach for the prediction of mole fraction dependent acid dissociation ([Angew. Chem. Int. Ed. 2019, **58**, 3212-3216]). During his master studies he started to work in the field of molecular chirality and optical activity. In his M.Sc. thesis, he investigated and developed static and dynamic approaches for the calculation of vibrational circular dichroism spectra in the liquid phase ([J. Phys. Chem. B 2020, **124**, 7272-7283], [Adv. Theory Simul. 2021, **4**, 2000223]). He continues this work in his Ph.D. project and uses the developed methods to investigate chiral phenomena (e.g., chirality transfer) in the condensed phase ([J. Org. Chem. 2022, **87**, 1867−1873]).