ADVANCING DYNAMIC METHODS FOR COMPUTATIONAL SPECTROSCOPY IN THE GAS AND CONDENSED PHASE

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I will give an overview about our work on development of novel computational methods for spectroscopy with emphasis on dynamic methods and approaches for the condensed phase.

I will describe the efficient calculation of Infrared spectra for periodic systems using subsystem density functional theory (DFT) as well as Raman and sum frequency generation spectra by means of DFT-based molecular dynamics. This has allowed a realistic description of (large) compounds including finite temperature and environmental effects. Moreover, pioneering Raman optical activity spectra for the investigation of chiral compounds using DFT-based molecular dynamics have been presented and a novel approach for vibrational circular dichroism. In addition, I will show our developments for excited state dynamics and using real time propagation for the study of absorption and vibrational spectra for (chiral) compounds in the gas and condensed phase.