Recent developments in dynamic spectroscopic methods for the gas and condensed phase

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Spectroscopy is an indispensable tool for the analysis of compounds. Calculations provide valuable insight and allow the targeted study of specific structures, their dynamics and interactions.

We present innovative methods for the calculation of spectroscopic signatures based on real time propagation as well as density functional theory-based molecular dynamics (DFT-MD) with a focus on vibrational spectroscopy. Besides the study of solvation effects [1,2,3], efficient DFT-MD approaches for Infrared and Raman spectroscopy for condensed phase systems [4,5], relying e.g. on periodic subsystem density functional theory [4], have been presented. Other developments have dealt with DFT-MD for Sum Frequency Generation and Raman Optical Activity spectroscopy [6,7]. Moreover, innovative analysis methods have been presented [4,5,8]. This has paved the way for the computationally efficient and accurate study of molecules on (semiconductor) surfaces/interfaces and in gas/liquid phase at ambient conditions with consideration of anharmonicity and realistic band shapes in the spectra. Among various investigated systems, chiral ionic liquids have been explored in detail [9]. Another direction has concerned the use of real time propagation for linear spectroscopy and excitation profiles in vibrational spectroscopy [10].

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