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Recent advances in theoretical spectroscopy from *ab initio* molecular dynamics

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Knowledge about properties of liquid is extremely helpful for the analysis of molecular structures and interactions. Moreover, it is a valuable source of information for the characterization of dynamic processes and facilitates the interpretation of experimental data. Calculations provide additional insight allowing the targeted study of specific structures. In this way, it is possible to quantify the contributions of, e.g., solute and solvent molecules or adsorbates on solids. We present innovative methods for the calculation of spectroscopic and local properties for periodic systems such as liquids, which can efficiently be employed in density functional theory-based molecular dynamics. Moreover, computationally efficient approaches for the calculation of Raman and sum frequency generation spectroscopy have been developed as well as the first method for Raman optical activity spectroscopy from *ab initio* molecular dynamics. Recently studied systems include a gas-semiconductor interface as well as ionic liquids.

Biography

Sandra Luber completed her MSc and PhD degree from ETH Zurich in 2007 and 2009, respectively. After Post-doctoral studies at University of Basel and Yale University, she joined BASF SE in 2012. Afterwards, she became Project Group Leader at University of Zurich. Her Habilitation thesis was completed in 2016 and she is currently an SNSF Professor at University of Zurich.

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