Revealing Solvent Effects on Chromophore Vibrational Spectra: Dynamic Insights from DFT/MM and Time-Series Analysis

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Understanding vibrational response of molecules in solution is crucial for various applications. However, accurately modeling these spectra requires accounting for environmental influences, emphasizing the importance of explicitly taking into account the environment with a hybrid DFT/MM approach.

By conducting a time-series analysis of dipole moment and polarizability tensor along a DFT/MM trajectory[1], we successfully model the vibrational Infrared (IR) and Raman spectra of organic chromophores derived from the triangulenium dyes family, specifically ADOTA^+ in aqueous solution[2]. Additionally, we extend our study to the Tata-Octyl molecule, comparing computational results to experimental spectra. Through comparative analyses with gas-phase and static-level spectra, we elucidate solvent-induced alterations in vibrational behavior, providing insights into solvent effects and anharmonicity.

Our work not only enhances our understanding of vibrational properties in solution but also highlights the potential of machine learning to accelerate DFT/MM simulations, offering a robust framework for future studies in this field.

Keywords: ab initio Molecular Dynamics; Hybrid Density Functionals; Time Series Analysis; Vibrational Spectra.

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