DFT-based molecular dynamics simulations for the interpretation of gas phase IR-MPD experiments of floppy peptides and for condensed phase IR experiments

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Finite temperature DFT-based ab initio molecular dynamics simulations are presented for the calculation of infrared spectra in relation with IR-MPD experiments (InfraRed MultiPhoton Dissociation exps). Illustrations are taken from our recent works on flexible peptides of increasing size and complexity in relation with IR-MPD experiments. A special emphasis will be put forward on the importance of taking the effect of conformational flexibility into account in the calculation of the spectra as well as taking into account vibrational anharmonicities, all properties that are naturally included in molecular dynamics simulations.

We also present our new method for extracting "Effective Normal Modes" from the dynamics, more specifically with the goal of assigning the active vibrational modes from the simulations in terms of internal movements. Illustration of the method for extracting mode couplings anharmonicities will also be presented.

We will also show how all the methodology can be applied to liquid phase spectra calculations with illustrations from our works on peptide models, as well as on solid/liquid interfaces.

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