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Infrared spectra of small biomolecules from first-principle molecular dynamics simulations and effective normal mode analysis

First-Principle Molecular Dynamics (FPMD) has been recognized lately as a powerful tool to compute infrared spectra of a variety of systems. The main advantage of this approach with respect to the usual normal mode analysis approach at the optimized geometry is the explicit treatment of temperature and environmental effects, without need for an harmonic approximation. However, the interpretation of the simulated spectra in terms of atomic motions, phonons or vibrational modes is still a challenge: the vibrational modes have to be extracted from the computed trajectory instead of being computed individually as in the standard normal mode calculations. We propose the interpretation of the computed spectra using effective normal modes, constructed as the modes most localized in frequency. We show the analogy between these modes and the standard normal modes, towards which the effective normal modes converge in the limit of low temperatures. We will then show examples of this strategy, FPMD plus effective normal modes, for the computation and interpretation of infrared spectra of small biomolecules both in solution and in gas phase (in relation to IRMPD) at finite temperature.