Semi-local calculation of IR spectra using linear response theory

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1 Abstract

Vibrational spectroscopy techniques are used to perform structural characterization of molecules, as well as macromolecules. In this respect, techniques like Infrared (IR), Raman and Vibrational Circular Dichroism (VCD). These techniques can be simulated by calculating the linear response function. These responses can come from a series of classical molecular dynamics (MD) simulations, employing a quantum mechanical molecular mechanical (QM/MM) force field, where observables such as dipole moment, magnetic dipole moment, and polarizability are necessary.
The methodology developed in this work, which was incorporated into the AMBER 11 suite, uses semi-empirical like AM1, PM3 and Density Functional Tight Binding quantum method.
First, an α-helix was used to validate the Infrared spectroscopy simulation method. It was shown that it is possible to start with a classical MM potential surface to equilibrate the molecule at the desirable temperature, and move to a QM/MM potential surface for its production stage, using a reasonable equilibration time. In the same way, it was shown that the simulation does not have to be very long in order to get a good spectrum, and that it is possible to perform a parallel calculation of the spectrum by using different structures as starting points, which are obtained from a MM MD simulation.
For the second case the same methodology was employed to calculate the semi-local IR spectrum of eight amino acids inside of a α-helix, which consists of 18 Ala residues. These 8 residues were simulated by using QM theory while the remaining residues were simulated with MM. Constraints over dihedral Ψ and Φ dihedral angles were kept in order to conserve the structure.

So far, the results obtained in the case of IR spectroscopy show promising results for the successful application of the methodology on biomolecules. Therefore, this exploration is likely to provide more information about the molecules of interest, which can prove helpful in understanding and interpreting experimental results.