Water and Aqueous Solutions According to Molecular Dynamics Simulations

In this practical we will focus on the study of IR spectra of different water models and of glycine in aqueous solution. It is extremely difficult to build a water model that reproduces all of the properties observed in experiments equally well. Naturally, by now, there are several different water models that are capable of mapping certain properties of water very accurately while others are almost neglected. We will compute the IR spectra of some of the commonly used models (SPC, TIP3P, TIP4P and flexible TIP4P) in order to show the capabilities and limitations of these models in reproducing the IR responses.
The spectra will be compared to *ab initio* results. In the second part of the practical we will look at glycine. Glycine is a biomolecular building block (for proteins) which makes its analysis an important case study for the interactions with water. We will compute the IR spectrum of glycine in aqueous solution via force field MD simulations which will illustrate the concept and the difficulties of theoretical computations of solvated systems and the limitations of force field molecular dynamics. Further we will discuss the interactions of water with glycine based on ab initio results.