

Water and Aqueous Solutions According to Molecular Dynamics Simulations

The participants will be introduced to classical Molecular Dynamics simulations and the theoretical background of how to compute fully anharmonic vibrational spectra based on these simulations. In the course of the practical each participant will set up his/her own simulation of pure water and an aqueous solution of glycine followed by the computation of the IR-spectra. Different water models are used for the classical simulations and are compared to ab initio simulations. At the end of the practical, participants will have an understanding of the work flow of setting up a simulation for spectral computation and the difference between force field and ab initio simulations.