Introducing TRAVIS

We present TRAVIS ("Trajectory Analyzer and Visualizer"), a free program package for analyzing and visualizing Monte Carlo and molecular dynamics trajectories. The aim of TRAVIS is to collect as many analyses as possible in one program, creating a powerful tool and making it unnecessary to use many different programs for evaluating simulations. This should greatly rationalize and simplify the workflow of analyzing trajectories. TRAVIS is written in C++, open-source freeware and licensed under the terms of the GNU General Public License. It is easy to install (platform independent, no external libraries) and easy to use. [1]

Fig. 1: Snapshot of a Molecular Dynamics Trajectory

On this poster, we present some of the algorithms that are implemented in TRAVIS - many of them widely known for a long time, but some of them also to appear in literature for the first time. All shown analyses only require a standard MD trajectory as input data.

Theory meets Experiment

We apply our newly developed method to obtain spectra of methanol in vacuum (Fig. 5a) and of neat methanol in the liquid phase (Fig. 5b). Both spectra are based on an ab initio molecular dynamics simulation and therefore include anharmonicities. The simulations took approx. 2 weeks of computational time on 8 cores per simulation, which is acceptable for the calculation of high-quality bulk phase spectra. [2]

Our results nicely coincide with experimental spectra taken by the Vöhringer group. The typical bulk phase behavior is reproduced (e.g. broadening and red-shift of the O-H stretching band due to hydrogen bonding in the liquid).

Spectra from Molecular Dynamics

A widely used approach to obtain molecular vibrational spectra relies on the calculation of normal modes as a first step. This is mostly done within the harmonic approximation, which assumes that the potential surface behaves completely harmonic – this is often not the case. Apart from that, this methodology only works well for isolated molecules in vacuum or small clusters. Solvent and bulk phase effects cannot be captured.

The approach we present here enables the calculation of IR and Raman spectra based on ab initio molecular dynamics. The spectra are obtained as fourier transform of autocorrelation functions of certain quantities along the trajectory (Dipole Vector for IR, Polarizability Tensor for Raman). This method does not rely on the harmonic approximation and includes many anharmonicity effects of the systems investigated. Apart from that, full solvent influence is captured within the spectra. This enables accurate computation of liquid bulk phase spectra, which is not possible within the standard approach.

Voronoi Tessellation

Voronoi Tessellation of chemical bulk phase systems offers a great way to define neighborhood without any bias (like e.g. with distance criteria, like usual). The tessellation method is strictly defined and does not possess any parameter which could be varied. An arbitrary point in space belongs to the Voronoi polyhedra of the atom to which it is closest (see Fig. 6). The calculation of the Voronoi Tessellation in 3D periodic boxes is a non-trivial task. We included the required algorithms in TRAVIS (based on Voron++ by Chris Rycroft). By applying this methodology to several bulk phase simulations, we were able to gain insight into the topological neighborhood structure (Fig. 8 and 9).