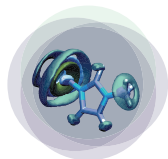


Trajectory post-processing with TRAVIS



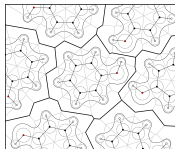
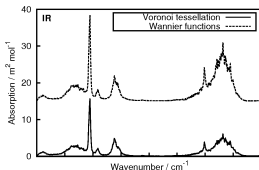
TRAVIS
TRAJECTORY ANALYZER
AND VISUALIZER

About

- open-source freeware tool
- all kinds of Molecular Dynamics or Monte Carlo simulations
- easy to install and easy to use

Features

- **Time independent functions**
distribution functions, structure factor, density profile
- **Time dependent functions**
velocity distribution or autocorrelation, diffusion coefficient
- **Spectroscopic functions**
Power, IR, and Raman spectra, normal mode analysis
- **Other functions**
cluster analysis, Voronoi tessellation, domain analysis



More info:

- <http://www.thch.uni-bonn.de/travis>
- M. Thomas, B. Kirchner, *J. Phys. Chem. Lett.* **2016**, 7, 509-513.
- M. Thomas, M. Brehm, B. Kirchner, *Phys. Chem. Chem. Phys.* **2015**, 17, 3207-3213.
- M. Brehm, B. Kirchner, *J. Chem. Inf. Model.* **2011**, 51 (8), 2007-2023.