



Bachelor thesis

Parallelization of computation for simulations of molecule-control experiments

The Controlled Molecule Imaging group at the Center for Free-Electron Laser Science at DESY and University of Hamburg performs novel experiments on the control and imaging of gas-phase molecules and their intrinsic ultrafast dynamics. We develop unique experimental approaches to record movies of molecules at work.

These novel experimental approaches are supported by computational simulations based on solutions of the time-dependent Schrödinger equation. To increase the accessible molecular complexity in these simulations we are implementing and improving parallelized solvers in our codes.

We offer a bachelor thesis project to perform an extended runtime analysis and implement corresponding performance improvements and significant parallelization of our TDasyrot program suite.

A successful candidate will have a strong background in modern software development. Experience in quantum physics, numerical methods, and massive parallelization are a plus.

We offer unique research opportunities in an interesting and open team and with first-class experimental and computational facilities. Our group is embedded in the Center for Free-Electron-Laser Science, DESY, the University of Hamburg and the excellence cluster Hamburg Center for Ultrafast Imaging.

Phys. Rev. Lett. 102, 023001 (2009) – <http://dx.doi.org/10.1103/PhysRevLett.102.023001>

Comp. Phys. Comm. 185, 339 (2014) – <http://dx.doi.org/10.1016/j.cpc.2013.09.001>

Phys. Rev. Lett. 114, 103003 (2015) – <http://dx.doi.org/10.1103/PhysRevLett.114.103003>

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Established by the European Commission

