FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

Zentralinstitut SCIENTIFIC COMPUTING

FRASCAL GRK 2423

BACHELOR THESIS

P12 Molecular Modelling of Fracture in Epoxy Resins

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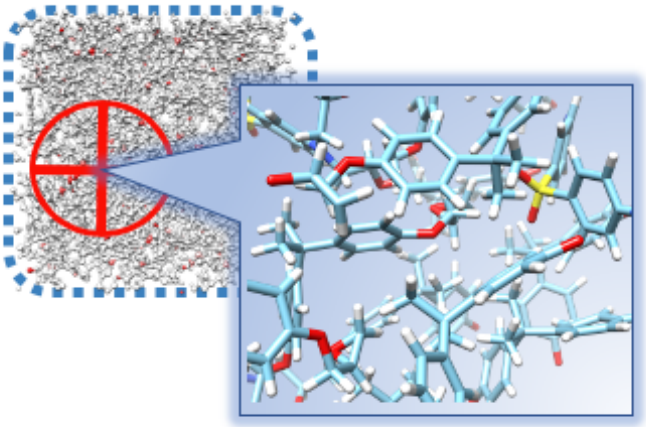

Hybrid QM/MM

Start Date: Anytime
Scientific Areas: Physics, Chemistry, Molecular Sciences, Material Physics and related fields

The Project: Modelling of Fracture in Epoxy Resins at the Molecular Scale
Epoxy resins are important thermosetting polymers of our everyday life with a large variety of applications such as structural materials in airplanes, as coatings and flooring materials in ships, cars and houses or as adhesives. Mechanical fracture of epoxy resins ultimately leads to the rupture of chemical bonds between the atoms of the covalently cross-linked polymers. However, the accurate description of the bond breaking process limits the applicability of classical molecular mechanical (MM) potentials to model the epoxy resins at the atomic level in e.g. molecular dynamics (MD) simulations. Quantum mechanical (QM) approaches are necessary to accurately describe the breaking of covalent bonds and related chemical change. We are developing QM/MM approaches which combine both worlds in order to understand the bond breaking process in epoxy resins at the molecular scale.

You are a bachelor student with a high interest in understanding complex processes at the molecular scale and want to be part of an interdisciplinary group. You are highly motivated and want to gain knowledge about state-of-the-art computational methods and tools.

Environment: The PULS group lead by A-S. Smith, Prof. for theoretical Physics is located at the new Interdisciplinary Center for Nanostructured Films (IZNF), which provides exquisite working conditions. The PULS develops and applies computational models and methods to study the effects of various physical and chemical phenomena at different length and time scales. We adapt and develop concepts and approaches of theoretical physics and computational chemistry to combine these with a variety of simulation techniques and experiments performed by us or by our collaborators. The project is strongly connected to the GRK 2423 - **FRASCAL**, which provides excellent training by experts in the field of computational modelling of fracture on multiple scales and includes a comprehensive program for soft skill seminars and mini-lectures.

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