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## **P12 Molecular Modelling of Fracture in Epoxy Resins**

**Contact:**

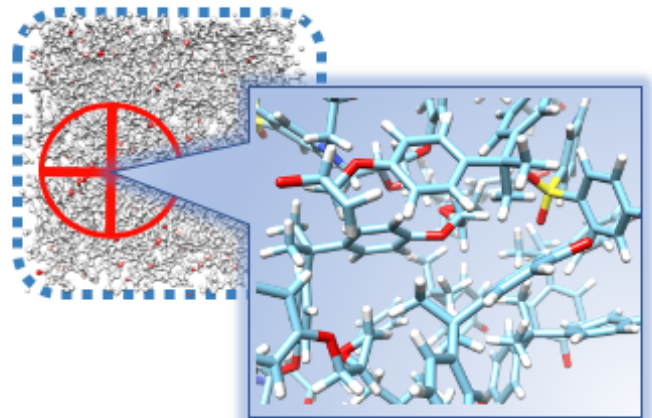
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**Start Date: Anytime**

**Scientific Areas:** Physics, Chemistry,  
Molecular Sciences, Material Physics and  
related fields



Hybrid QM/MM

**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** highly motivated and want to gain knowledge about molecular modelling tools, such as molecular dynamics simulation, force fields or quantum chemistry.

**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.



FRASCAL P12  
SCAN ME