Theoretical Chemistry

Molecular Modeling

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Project suggestions

These projects can be adjusted to fit a 15 (specialization project), a 30 or a 60 ECTS credit assignment. The research in the group ranges from applied quantum chemistry to the development of classical models for electronic polarization as well as molecular dynamics simulations of condensed phases. The projects may include method development, software development, or only calculations within a specific application area. The project descriptions below describe more a theme/research area of interest rather than one specific M.Sc. project. The individual project will be defined together with the student. A suitable background is the course TKJ4205 Molecular Modeling, which can be taken in parallel with a project.

1. Electrical insulation

We have a long-term collaboration with SINTEF Energy and ABB Corporate Research in Västerås, Sweden to understand electrical breakdown in liquids at an atomistic level. We are interested in molecular electronic processes at high electric fields such as ionization energies, electron affinities and the breakdown into small molecular fragments. Normally we work with a combination of quantum chemical calculations to obtain rate constants for various processes as well as solving the rate equation by kinetic Monte Carlo simulations.

2. Catalysis: metal particle - molecule interactions

In several research fields, it is of high interest to accurately model interactions between molecules and metal particles, and for this purpose we use density-functional theory (DFT) calculations. In collaboration with Prof. De Chen in the Catalysis group at NTNU, we study e.g. Pt and Co clusters on carbon support materials like graphene and how the interactions with the carbon material affect the catalytic activity of the metal atoms. In addition, we study molecule-coated nanoparticles, e.g. gold particles, which are important for applications in optics (with Fernando Bresme, Imperial College London).

3. Non-linear optics and electrical conductivity

We work on establishing “classical” models for electronic polarization and electron transport processes like the conductivity based on classical electromagnetism and concepts from force fields such as polarizabilities as well as relating these models to quantum mechanics. This type of projects is more “theory-oriented” and may also involve software development in addition to calculations. For validation and parametrization of the models, we use quantum chemical calculations. Optical properties that we are currently interested in includes nonlinear spectroscopy at interfaces (also with F. Bresme) as well as models for the molecular conductivity. A project along these lines may also be carried out in collaboration with the group at the University of Copenhagen that has an expertise in “molecular electronics”.