Master thesis project theme: Deep Earth materials and dynamics

Mineralogy and geochemistry of the lower mantle and core by atomistic simulations

Contact: Reidar Trønnes, Chris Mohn, John Brodholt or Razvan Caracas

E-mail: r.g.tronnes@nhm.uio.no, c.e.mohn@geo.uio.no, j.brodholt@ucl.ac.uk, razvan.caracas@ens-lyon.fr

Websites: www.nhm.uio.no/om/organisasjon/forskning-samlinger/personer/rtronnes
www.mn.uio.no/geo/english/people/aca/ceed/chrism/index.html
www.ucl.ac.uk/earth-sciences/people/academic/prof-john-brodholt#2018
http://razvancaracas.info/

Understanding the evolution and dynamics of the deep Earth and other planets requires data on minerals, melts and fluids at very high pressures. Because experiments at very high pressure and temperature conditions are difficult, an alternative and invaluable route for obtaining such data is through atomistic simulations. For instance, atomistic calculations have been essential for insights into the core-mantle boundary region with pressure and temperature ranges of 100-140 GPa and 2500- 4000 K. Atomistic computations have also provided constraints on the composition of the core, the mineralogy and phase relations in the mantle, the properties of melts and their evolution from a magma ocean until today, as well as the properties of exoplanets. The access to large computational resources and appropriate molecular dynamics software, has made ab initio theoretical studies a very attractive approach during the last ten years. The computing power has increased to the point at which studies of phases with complex solid solutions are feasible.

The deep Earth materials group at CEED, coordinated by Reidar Trønnes, includes research associate Chris Mohn and postdoctoral fellows, as well as two adjunct professors, John Brodholt at University College, London and Razvan Caracas, CNRS, Ecole Normale Superior, Lyon. We can offer a variety of MSc-projects to address exiting and unsolved issues related to deep Earth mineralogy, geochemistry and dynamics. The students will learn to use ab initio methods, which are highly sought-after skills in both academia and industry, and will have access to and gain skills in using high-performance computers.

Specific projects suggestions:

- Modeling of grain boundaries and their influence on crystal growth and mantle rheology.
- Modeling H diffusion in mantle silicates; predicting experimental observables.
- Deep Earth evolution and isolated reservoirs based on trace element partitioning between minerals and melts.
- Core and deep mantle evolution driven by silica crystallisation in the system Fe-Si-O.
- The silica phase transition from seifertite to a pyrite-structured phase at about 270 GPa.
- Si and Fe isotope fractionation around major boundaries of the deep Earth.
- Rheology of planetary ices: understanding the interior of Pluto at the atomic scale.
- Characterization of major boundaries inside super-Earths.
- Development and use of Monte Carlo methods along with DFT to understand disordered mantle minerals.
- Development and use of AI to predict new exotic minerals (e.g. in Mercury, super-Earths, etc.).