

Master thesis project theme: Deep Earth materials

Projects 1-4: Mineralogy and mineral physics of selected lower mantle minerals by first principles molecular dynamics (FPMD)

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FPMD-investigations represent a valuable route to insights in phase relations, p-V-T equations of state (EoS) and thermal conductivity of lower mantle minerals in either basaltic or peridotitic compositions. The resulting data provide constraints on seismological properties and mantle convection. The core-mantle boundary (CMB) region represents the most pronounced thermal boundary layer in the Earth, with temperature decreasing from about 4000 to 2500-3000 K over the lower 200-300 km above the CMB (the D"-zone). The material properties of the laterally and radially heterogeneous and structurally complex D"-zone zone is a main governing factor for global convective dynamics and Earth evolution. Technological challenges and problems related to experiments at conditions of the D" layer, combined with an easy 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 recently increased to the point at which studies of phases with simple solid solutions are feasible. We are currently studying the phase relations and partitioning of two Fe-bearing components, FeSiO₃ and FeAlO₃, in MgSiO₃-based perovskite and post-perovskite. The Earth's most abundant mineral, Mg-perovskite, transforms to the higher pressure form, post-perovskite, in the coolest regions of the D" zone. The investigated thermoelastic properties and thermal conductivity of these phases are fundamentally important for the dynamics of the CMB boundary region.

Similar investigations that may be suitable as MSc-projects include:

1. The partitioning of Al₂O₃ and MgAlO_{2.5} in MgSiO₃-based perovskite and post-perovskite
 2. The incorporation and substitution mechanism for Na₂O in MgSiO₃-based perovskite and post-perovskite. Reconnaissance experiments have indicated strong and largely enigmatic partitioning of Na₂O into post-perovskite.
 3. The partitioning and substitution mechanism for Al₂O₃ in the SiO₂-dominated phases in the lowermost mantle. A post-stishovite silica phase with the CaCl₂-structure is stable in basaltic lithologies along the entire lower mantle geotherm to about 2500 km depth and replaced by the higher pressure seifertite phase with the □-PbO₂-structure in the lowermost mantle. Reconnaissance experiments have indicated strong partitioning of Al₂O₃ to seifertite (12.6 wt%) relative to the CaCl₂-structured phase (3.4 wt%).
 4. The phase relations of the Al-rich phases in basaltic lithologies along selected binary join(s) in the system NaAlSiO₄-KAlSiO₄-MgAl₂O₄-CaAl₂O₄ at lower mantle condition. In the upper part of the lower mantle to about 1200 km depth a hexagonal phase (the new aluminous phase, NAL, space group P6₃/m) may coexist with an orthorhombic Ca-ferrite-structured phase (CF, space group Pbnm). The latter phase persists to the lowermost mantle (D") where it may be replaced by an orthorhombic Ca-titanite-structured phase (CT, space group Cmcm)
- All of these projects would involve the computation of thermoelastic properties (bulk and shear moduli, p-V-T equations of state) and thermal conductivity as a function of varying phase compositions.

Project 5: An *ab initio* computational study of the incorporation and diffusion of noble gases in major mantle minerals

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The isotope geochemistry of the noble gases measured in fresh basalts erupted in oceanic and continental settings puts important, although debatable, constraints on the origin and evolution of the source materials and therefore also on the deep Earth evolution. Although the main focus has been on the ³He/⁴He ratio, improved insights in chemical geodynamics require additional consideration of the behavior of other noble gases. The solubility, incorporation mechanism and diffusion rate of the noble gases in major mantle minerals like olivine, perovskite (especially Mg-perovskite, but also Ca-perovskite), post-perovskite and ferropericlasite are fundamentally important to understand the diffusional length scales (especially for the small He-atom) and the possibility of Hadean to present recharging of primordial He into depleted mantle domains (poor in He, U and Th) from either the ambient mantle or the outer core. Because our experimental technologies are largely inadequate to address these issues, the availability of increasingly larger computational resources makes first principles molecular dynamics a timely research avenue.