INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Room IC 02-722

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Deformation and defects in minerals: insights from atomic-scale simulations

The Earth is a hot planet that still dissipates its energy by large-scale convection movements in its mantle. This process occurs at the scale of millions of years, and is responsible for events that occur at the surface, such as earthquakes, volcanic activity, or plate tectonics. The constituents of the Earth mantle are solid rocks, that are deformed in extreme creep conditions. Thus, the whole process of convection depends on the collective deformation of the minerals that constitute the mantle.

We propose a bottom-up approach that relies on the study of elementary mechanisms at the atomic scale, and that aims towards phenomenological laws. To that end, atomic-scale simulations are performed in idealized minerals. They reveal that dislocation glide is a predominant mechanism in some phases, but can be completely inhibited in some other phases. In the latter case, deformation has to occur through different mechanisms, such as diffusion, dislocation climb, or grain boundary activity.