Title: **Atomistic mechanisms and kinetics during phase transformations in metals**

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Abstract:

Atomistic modelling of the dynamics of phase transformations is a particularly challenging task. If the mechanism of the phase transformation is governed by so-called rare events then the time scale of interest will reach far beyond the capabilities of regular molecular dynamics simulations.

One example are the atomistic rearrangements during solid-solid phase transformations in bulk systems which involve massive structural changes including concerted multi-atom processes. The interface between two structurally different phases leads to a complex energy landscape that needs to be exploredduring the dynamical evolution of the interface. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach to investigate such processes at the interface between the body-centered cubic and A15 phase in molybdenum.

A second example is the initial nucleation and growth during solidification in metals. Here, we investigate the atomistic mechanisms of nucleation in nickel for various undercoolings using transition path sampling (TPS). The analysis of the path ensemble reveals a non-classical behaviour with mainly non-spherical nuclei, and shows that the nucleation initiates in regions with high orientational order that also predetermine the polymorph selection.