MAX-PLANCK-INSTITUT
FÜR DYNAMIK KOMPLEXER
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CSC Seminar

SPEAKER

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TITLE

Predicting the solid-state atomic kinetics with uncertainty

ABSTRACT

I will discuss two methods to coarse-grain and predict molecular dynamics simulations, with a focus on solid-state diffusion and plasticity.

First, I will show how metastable diffusive kinetics can be rigorously mapped to a discrete Markov chain with robust Bayesian bounds on as-yet unseen transitions. These bounds are used to allocate resources in massively parallel computation and measure the convergence of coarse-grained transport properties[1].

However, in many important cases, in particular plastic deformation, kinetics show no clear signature of metastabilty. I will discuss how many-body basis functions used in atomic machine learning form a metric latent space ideal for coarse-graining and analysis. A vector autoregressive model can resample and forecast latent space trajectories using a Mahalanobis distance to qualify forecast uncertainty, with the descriptor manifold clearly sensitive to structural transitions[2].

[1] TDS and D Perez, NPJ Computational Materials 2020
[2] TDS, under review at PRL, 2023

Wednesday, November 22, 2023 at 10:00 am
seminar room Prigogine