NOMATEN HYBRID-JUNIOR-SEMINAR

online: https://www.gotomeet.me/NCBJmeetings/nomaten-seminar
In-person: Proton 251,PNT, seminar room, PNT, NCBJ

Thursday, OCTOBER 13th 2022 13:00 (1.00PM CET)

Fast and accurate machine-learned interatomic potentials for refractory metals and alloys

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Abstract:

Refractory high-entropy alloys possess good high-temperature strength and have shown promising tolerance to irradiation, yet much is still unknown about the atom-level mechanisms that control the mechanical properties and the consequences of irradiation. This is largely due to the difficulties of accurate atomistic modelling of alloys with many elements. For molecular dynamics simulations, developing interatomic potentials is challenging due to the vast configuration space that needs to be sampled by the fitting data. I will demonstrate that simple machine-learned interatomic potentials based on low-body descriptors for the local atomic environments can achieve remarkable accuracy for refractory Mo-Nb-Ta-V-W alloys. The potentials are based on the Gaussian approximation potential framework (GAP) and subsequently tabulated and evaluated using cubic splines (tabGAP), yielding a speedup of two orders of magnitude. The potentials contain accurate repulsive parts that make them applicable to radiation damage simulations. In the seminar, I will briefly discuss the potential development, and then show results of simulations of short-range ordering, segregation, diffusion mechanisms, and radiation response of the equiatomic MoNbTaVW alloy.

Bio:

Dr. Jesper Byggmästar is a postdoctoral researcher at the University of Helsinki and the Finnish Center for Artificial Intelligence. He defended his PhD in 2020 on the topic of radiation damage modelling and interatomic potential development for fusion-relevant materials. Two years after completing the PhD, he has published 30 peer-reviewed papers. His specific expertise is on developing both analytical and machine-learning interatomic potentials, with 14 papers on the topic of which 9 as first author.