Institute for Materials Science
Universität Stuttgart

Colloquium
Materials Science
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On-line per WebEx !
Meeting number: 121 506 8121
Meeting password: UniSMaWi

Meeting link:
https://kurzelinks.de/MaWi-UniStuttgart

"Towards automated potential development: applications to thermoelectrics, molten salts, shape-memory-alloys, and high-entropy-materials"

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Abstract:
Molecular dynamics (MD) simulations using classical or machine-learned interatomic potentials have an integral role in the modelling of materials where relevant length- and time-scales too large to treat directly using ab initio approaches such as density functional theory (DFT). A critical challenge in leveraging MD however is the development of reliable potentials.
By now, many of the steps in developing an interatomic potential are highly automated. First, there is the ready availability of density functional theory (DFT) codes with which to generate reliable training data. Second, given such data, potential-optimization codes like MEAMfit can automatically fit an interatomic potential with minimal user intervention. The remaining bottle-neck however, and that which still requires expert guidance, is deciding what DFT data to use, I.e., the 'training set', to optimize a given potential.
To address the challenge we are designing an 'Automated potential development (APD)' toolkit which addresses not only the challenge of defining the training set, but moreover provides a workflow for automating as far as possible the potential development process as a whole.
In this talk we discuss the APD, and applications to tetrahedrite, a thermoelectric material, and molten sodium chloride, relevant to molten salt reactors and energy storage. We will also present some other applications of MEAMfit (not related to the APD) including: shape-memory-alloys and high-entropy-materials.

Host: Prof. Dr. Blazej Grabowski