EMPLOYING AB INITIO THERMODYNAMICS TO DESIGN STRUCTURALLY COMPLEX MATERIALS

Neugebauer J.,* Zhu L., Körmann F., Grabowski B., Hickel T.

MPIE, Düsseldorf, Germany

**neugebauer@mpie.de*

Ab initio approaches provide in principle perfect tools for the design of new materials, but face serious challenges: Free energies which are the key quantity to compute thermodynamic phase diagrams, deformation paths or defect formation energies require formalisms that accurately capture all relevant entropic contributions due to electronic, vibrational or magnetic excitations, as well as their coupling such as phonon-phonon, magnon-phonon interactions or spin-quantization. Calculating these contributions is conceptionally challenging and computationally expensive. The talk gives an overview over the developed approaches and their ability to accurately describe thermodynamic quantities and phase transitions. Based on these studies the performance of popular DFT functionals in describing these quantities will be discussed. To demonstrate the practical applicability of these approaches examples will be given showing how they helped discovering a new class of light-weight metallic alloys with improved mechanical properties.