INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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From chemical stability to mechanical properties: Multi-scaling based on quantum mechanics

Due to their predictive power, methods based on electronic structure theory are more and more applied for modelling real materials properties within a quantum mechanical framework. From a technical point of view, the vision behind is the design of functional materials with special properties before expensive experiments are performed. We use density functional theory to calculate both free energies and various quantities of technological relevance. Of special interest are mechanical properties as elastic constants or Zener ratio, and their relation to phase stability quantified by order parameters of high-end materials like Ni-rich alloys or hybrid materials.
Based on the formalism of the cluster expansion [1] as realized in the UNCLE [2] package, it is possible to expand any configuration dependent observable like the formation enthalpy in terms of its manybody interactions.
These types of cluster expansion each yield the formation enthalpy plus one or more of the aforementioned other quantities. This enables us to relate e.g mechanical properties of a structure with its chemical stability.

[1] J. M. Sanchez, F. Ducastelle, D. Gratias: Physica 128 A, 334, (1984).
[2] D. Lerch, O. Wieckhorst, G. L. W. Hart, R. Forcade, S. M□uller: Modelling Simul. Mater. Sci. Eng. 17, 055003, (2009).