Vienna Computational Materials Laboratory

ViCoM

INVITATION TO A GUEST LECTURE

STEFAN MÜLLER, HAMBURG UNIVERSITY OF TECH.

Dear Colleague,

we cordially invite you to the following guest lecture in the scope of our workshop from 28th of April 2011 – 29th of April 2011. Thank you.

STEFAN MÜLLER – HAMBURG, GERMANY
Professor, Institute Advanced Ceramics, Hamburg University of Technology (TUHH)

Presentation Title

"Non-scalar Cluster Expansions for Arbitrary Configuration Dependent Observables" (35-40 min.)

Date, Time & Location

"Christian-Doppler-Lecture Hall" (Faculty of Physics, University of Vienna – Boltzmanngasse 5/Strudlhofgasse4, 3rd Floor, A-1090 (9th District) Vienna, Austria)

Friday, 29.04.2011, 09:40 – 10:20

Abstract

Sascha B. Maisel, Nils Schindzielorz and Stefan Müller – Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungs-werkstoffe, Denickestr. 15, D-21073 Hamburg, e-mail: stefan.mueller@tuhh.de

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 DFT-based approaches to calculate both free energies and various quantities of technological relevance for a giant number of atomic configurations. Of special interest are mechanical properties as elastic constants, bulk moduli or Zener ratio, and their relation to phase stability quantified by order parameters of high-end materials like Ni-rich alloys. 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 many-body interactions. In this talk, we present several cluster expansions performed for multiple observables simultaneously. 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. Supported by DFG.

[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. Müller: Modelling Simul. Mater. Sci. Eng. 17, 055003, (2009).