TECHNISCHE UNIVERSITÄT CHEMNITZ

PHYSIKALISCHES KOLLOQUIUM

Mittwoch, 27.11.2013, um **17:15 Uhr**

Ort: Reichenhainer Str. 90; Neues Hörsaalgebäude, Raum: 2/N013

Prof. Dr. Stefan Müller
Technische Universität
Hamburg-Harburg

From the atom to real materials properties: concept and realization

Although modern computer codes based on density functional theory (DFT) allow for the reliable prediction of many surface und bulk properties of solids, they cannot be applied, when the problem of interest demands a consideration of huge configuration spaces or model systems containing many thousand atoms. Examples are precipitation or segregation in alloys where substitutional ordering phenomena on a mesoscopic scale are involved. Moreover, in general DFT based methods do not permit us to study exchange processes between atoms and therefore, do not consider configurational enthalpies being a prerequisite for modeling the temperature-dependence of e.g. decomposition reactions. In this talk, recent developments, possibilities and limitations to study materials properties on different scales by use of first-principles methods will be discussed. It will be demonstrated, how the combination of DFT calculations with so-called Cluster Expansions and Monte-Carlo simulations allows for a quantitative prediction of materials properties from the microscopic to the macroscopic scale without any empirical parameters.

Alle Zuhörer sind ab 17:00 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt Prof. Dr. Thomas Seyller, Tel.: 0371 531 32898