O 9 Hauptvortrag Müller

Zeit: Freitag 14:45–15:30 Raum: TU EB301

Hauptvortrag O 9.1 Fr 14:45 TU EB301

Structure and stability of binary alloy surfaces: Segregation, relaxation, and ordering from first-principles calculations — •Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen

Although modern computer codes based on density functional theory (DFT) allow the reliable prediction of many surface properties, they often cannot be applied when the problem of interest demands a consideration of huge configuration spaces or model systems containing many thousand atoms. An important example are binary alloy surfaces where substitutional ordering phenomena on a mesoscopic scale and surface segregation are involved. The latter describes the deviation of the surface region's stoichiometry from that of the bulk. Consequently, a successful theoretical description of this phenomenon demands the consideration of both, bulk and surface properties leading to model slabs consisting of hundreds, if not thousands of atoms. Moreover, in general first-principles methods based on DFT cannot take configurational enthalpies into account and, therefore, are not able to describe the segregation of atoms at all. In this contribution, our recent developments, possibilities and limitations to study surface segregation and ordering phenomena in metal alloys based on 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 alloy surface properties from the miscroscopic to the mesoscopic scale without any empirical parameters (supported by DFG).