

O 17 Hauptvortrag Stampfl

Zeit: Samstag 09:45–10:30

Raum: TU EB301

Hauptvortrag

O 17.1 Sa 09:45 TU EB301

Order-disorder Surface Phase Transitions from First-principles

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One of the most important goals of theoretical surface science is to achieve an ab initio atomistic description that can predict phenomena and properties occurring on macroscopic length and long time scales [1]. Clearly, knowledge of the surface structure and composition are crucial ingredients for such a description. This talk will discuss through the example of Na-Al surface alloys, state-of-the-art first-principles based theoretical methodology and concepts which allow an accurate and fast predictive description of equilibrium surface structures and phase transitions as a function of temperature and stoichiometry [2]. The system is described using a lattice-gas Hamiltonian (LGH), together with Monte Carlo (MC) simulations. In addition to standard MC, the new MC algorithm of Wang and Landau [3] is employed in which the density of (configurational) states are explicitly obtained. From this the thermodynamic quantities such as the free energy and entropy are directly determined.

[1] K. Reuter, C. Stampfl and M. Scheffler, Handbook of Materials Modeling, Volume 1, Fundamental Models and Methods, Sidney Yip (Ed).

[2] M. Borg, et al. to be published.

[3] F. Wang and D.P. Landau, Phys. Rev. Lett. 86, 2050 (2001).