THEORIEKOLLOQUIUM & Sonderkolloquium SFB/TRR80

Freitag, den 20.04.18 um 12:00 in MC 351

PD Dr. Volker Eyert

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Materials Design in Practice: Atomistic Simulations in Science and Industry

During the past decades, atomic-scale simulations have emerged as a tool of materials research and engineering both in academia and industry. Leading industrial research laboratories, public laboratories, and universities have started to combine experimental data with the predictive power and the key to understanding materials properties as offered by atomistic simulations to solve engineering problems connected, e.g. to long-term stability of materials or to identify novel and environment friendly materials. In this situation, as the computer power is tremendously growing, comprehensive computational environments, which take away the burden of routine tasks, are coming to the fore allowing researchers to focus on the scientific problem at hand. Using sophisticated model building and analysis tools, computational environments as the MedeA® software combine experimental structures and phase-diagrams with state-of-the-art computational procedures for property predictions for systems including alloys, semiconductors, ceramics, glasses, polymers, and fluids. Furthermore, these tools facilitate the simulation, e.g. of the electronic structure and mechanical properties, as well as the thermal behaviour for complex structures such as interfaces, heterostructures, grain boundaries, defect structures and random alloys. The comprehensive capabilities of such modelling tools will be illustrated by applications including the development of low-strain cathode materials for batteries, the analysis of grain-boundary stability in electronic devices, and the search for optimum materials for hydrogen storage in the automobile industry.

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