The Application of Ab Initio Electronic Structure Calculations in Multiscale Modeling of Materials

by

Professor Mojmír ŠOB
Department of Chemistry
Masaryk University, Czech Republic

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(Light refreshments will be served 20 minutes prior to the colloquium.)

ALL INTERESTED ARE WELCOME

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Abstract

Many properties of solids can be predicted accurately from the ab initio (first principles) electronic structure calculations, i.e. from the fundamental quantum theory. However, the state-of-the-art ab initio calculations are computationally very intensive and only relatively small number of non-equivalent atoms (up to 500-1000) may be relaxed. For more complicated cases encountered in micro-mechanical engineering problems, e.g. for atomistic studies of mechanical properties of real materials containing dislocations, we have to resort to simpler methods using semiempirical interatomic potentials with adjustable parameters, such as Finnis-Sinclair potentials, embedded atom method, bond-order potentials, or model generalized pseudopotential theory. To get reliable interatomic potentials, experimental data are usually not sufficient and one must include into the fitting procedure also some high-energy configurations the properties of which can be calculated by ab initio methods.

In the present talk, the ab initio electronic structure calculation methods will be reviewed briefly and their applications in multiscale modeling will be illustrated on the following examples:

(a) segregation of Bi at grain boundaries in Cu
(b) structure of grain boundaries in Ni and analysis of the positron annihilation signal
(c) theoretical strength of metals and intermetallics.

Enquiries: 2609 6339