Seminář odd. 26
Tenkých vrstev a nanostruktur

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Ali Sadeghi

Physics Department, Swiss Nanoscience Institute, University of Basel

Part 1: Minima Hopping Method: Structure prediction of nano-systems

The global minimum of the potential energy surface (PES) determines the ground state configuration of any condensed matter system. In a global geometry optimization one faces the difficulty that the number of local minima increases exponentially with the system size. Minima Hopping is a powerful and unbiased global geometry optimization method with the advantage of efficiently avoiding search over unnecessary regions of the potential energy landscape thanks to being based on fundamental physical principles. The algorithm and some results on different nano-systems including clusters, nano-structures and biomolecules will be presented.

Part 2: Multiscale simulation of Kelvin probe force microscopy

The distance dependence and atomic-scale contrast in Kelvin signals recently observed with nc-AFM on conducting, as well as on insulating samples has stimulated theoretical attempts to explain these effects. We attack the problem in two steps: 1) The macroscopic electrostatic potential and the capacitance between the tip+cantilever system and the thick insulating sample are determined; 2) The microscopic site-dependent electrostatic force are performed within the wavelet-based BigDFT code. The local contact potential difference is then defined considering the both contributions.

odborný garant: *Ing. Pavel Jelínek, Ph.D.*