Seminář odd. 26
Tenkých vrstev a nanostruktur

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

datum: 1. 11. 2016 úterý

čas: 10:00

místnost: knihovna, budova A, 1.p.

TÉMA

Towards an accurate theoretical description of extended systems

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Computational modelling has been very useful in helping to understand adsorption, catalysis, high pressure phases of materials, and many other systems. For reliable description of such systems and processes, accurate methods are required. Unfortunately, the current workhorse for many such studies, the density functional theory (DFT) approximations, have limited accuracy and sometimes can lead to even qualitatively incorrect results. The random phase approximation (RPA) is a promising candidate for the next method for simulations of extended systems. With recent algorithmic improvements, it can now be applied to systems with hundreds of atoms in the unit cell, such as molecular solids or surfaces with adsorbed molecules. Moreover, we have recently substantially improved the accuracy of RPA so that in many cases it comes within few percent of the available reference binding energies. Finally, reliable data also need to be precise, i.e., converged with the parameters of the numerical set-up. I will discuss the recent developments of RPA as well as some of the issues that one encounters when trying to obtain reliable data and possible ways for solving them.

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