Ústav fyzikální chemie Jaroslava Heyrovského
Akademie věd České republiky

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zve všechny zájemce na ústavní seminář, na kterém promluví

Prof. Jürgen Hafner

(Institute for Materials Physics, Vienna University)

na téma

Ab-initio simulations of materials using VASP - density-functional theory and beyond

Seminář se koná **ve středu 15. listopadu 2006 od 10 hodin.**

ve velké posluchárně ústavu v Praze 8, Dolejškova 3.

Těšíme se na Vaši účast. Hosté jsou vítáni.

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Ab-initio simulations of materials using VASP - density-functional theory and beyond

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The development of modern materials science has led to a growing need to understand the phenomena determining the properties of materials and of processes in materials on a truly atomistic level. The interactions between atoms and electrons are governed by the laws of quantum mechanics and hence accurate and efficient techniques for solving the quantum-mechanical equations for complex many-atom, many-electron systems must be developed. Density functional theory (DFT) has marked a decisive breakthrough in these efforts, and the past decade has witnessed a rapidly growing impact of DFT not only on fundamental, but also on industrial research. In my contribution I shall discuss very briefly the fundamental principles of DFT and their implementation in an efficient software package, the Vienna ab-initio simulation package VASP and present a number of applications in key areas of materials science, ranging from complex metallic alloys over magnetic materials to catalysis.

However, DFT does not solve all problems - the "band-gap problem" (i.e.the difficulty to achieve a quantitatively accurate prediction of the gap between the highest occupied and the lowest empty eigenstate) and the inability to describe the physics of van der Waals interactions are notorious. Also the properties of strongly correlated systems such as transition-metal oxides are not well reproduced by DFT. Evidently the exploration of the many-body aspects of electron-correlation beyond current DFT methods is needed and I shall discuss the implementation of some such approaches (DFT+U, GW, hybrid functionals) in VASP, together with some front-line applications.