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Gegründet im Jahre 1869 von H. Hlasiwetz,
J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag von

Prof. Dr. Igor A. Abrikosov
Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

Materials at extreme conditions: from nanocomposites to Earth's core

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Dienstag, 12. Oktober 2010, um 17.00 Uhr

Ort: **Ernst-Mach-Hörsaal**, Fakultät für Physik, Universität Wien, **2. Stock**
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5 - ***bitte Hörsaal beachten***

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 2. Stock

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Abstract:
We will review recent developments in the field of *ab initio* electronic structure theory and its application for studies of complex materials at extreme conditions. Basic ideas behind state-of-the-art techniques for first-principles theoretical simulations of the phase stabilities and properties of intermetallic alloys at ultrahigh pressure and temperature will be outlined. We will concentrate on methods that allow for an efficient treatment of disorder effects [1], and illustrate their predictive power with examples.

Three major factors that determine the stability of alloy phases are the difference in size between the alloy constituents, the difference in their electronegativity, and the valence electron concentration. All of them can be tuned by compression, which opens up intriguing possibilities for the design of novel materials and optimization of their properties. We show that alloys between immiscible elements, like Fe and Mg, can be formed upon compression. We predict that hydrostatic pressure, which is actually present in cutting tool applications, enhances the tendency for isostructural decomposition in nanocomposite TiAlN thin films, used as hard protective coatings at the cutting tools. In Fe-Ni Invar alloys we discover the pressure induced Invar effect, and we demonstrate that by tuning the magnetic interactions at high pressure and temperature, we are able to synthesize Fe_2Si alloy with B2 crystal structure, not present at the phase diagram of this system. We show applications of the theory in studies of the crystal structure and composition of the Earth's core. At temperature of 5000-6000 K and pressure of 350 GPa three close-packed phases of Fe, hcp, bcc, and fcc, are very close in energy to each other, but alloying Fe with Ni favors the stabilization of the bcc phase, actually observed in experiments at extreme conditions [2].

[1] A. V. Ruban and I. A. Abrikosov, Rep. Prog. Phys. **71**, 046501 (2008).
[2] L. Dubrovinsky, N. Dubrovinskaia, O. Narygina, A. Kuznetzov, V. Prakapenka, L. Vitos, B. Johansson, A. S. Mikhaylushkin, S. I. Simak, and I. A. Abrikosov, Science **316**, 1880 (2007).