INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Thursday, 25th of November, 11:00 p.m.
ICAMS Seminar room UHW 11/1102

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Ab initio simulations of alloys: from nanomaterials to Earth's core

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.

Firstly, the ability of the theory to deal with nanosystems will be illustrated with an example of the self-consistent determination of segregation profiles in ultra-thin alloy films. In particular, we discuss the double-segregation effect in AgxPd1-x/ Ru(0001) thin-film nanostructures [2]. Secondly, we reveal the origin of the anomalous, 400% increase of the piezoelectric coefficient in ScxAl1-xN alloys. Quantum mechanical calculations show that the effect is intrinsic. It comes from a strong change in the response of the internal atomic coordinates to strain and pronounced softening of C33 elastic constant. The underlying mechanism is the flattening of the energy landscape due to a competition between the parent wurtzite and the so far experimentally unknown hexagonal phases of the alloy. Our observation provides a route for the design of materials with high piezoelectric response [3]. Finally, we show applications of the theory in studies of the crystal structure and composition of the Earths 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 [4].

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[2] T. Marten, O. Hellman, I.A. Abrikosov, A.V. Ruban, W. Olovsson, C. Kramer, L. Bech,L. J. Onsgaard, P. J. Godowski, Z.S. Li, Phys. Rev. B 77, 125406 (2008)
[3] F. Tasnadi, B. Alling, C. Hglund, G. Wingqvist, J. Birch, L. Hultman, and I. A. Abrikosov, Phys. Rev. Lett. 104, 137601 (2010).
[4] 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).