

On behalf of the
Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

Dr. Josef Kudrnovský

Institute of Physics AS CR, Czech Republic

**Magnetism of mixed quaternary Heusler alloys:
(Ni_{1-x}T_x)₂MnSn (T=Cu, Pd) as a case study**

The electronic properties, exchange interactions, finite-temperature magnetism, and transport properties of random quaternary Heusler Ni₂MnSn alloys doped with Cu- and Pd-atoms are studied theoretically by means of *ab initio* calculations over the entire range of dopant concentrations. While the magnetic moments are only weakly dependent on the alloy composition, the Curie temperatures exhibit strongly non-linear behavior with respect to Cu-doping in contrast with an almost linear concentration dependence in the case of Pd-doping. The present parameter-free theory agrees qualitatively and also reasonably well quantitatively with the available experimental results. An analysis of exchange interactions is provided for a deeper understanding of the problem. The dopant atoms perturb electronic structure close to the Fermi energy only weakly and the residual resistivity thus obeys a simple Nordheim rule. The dominating contribution to the temperature-dependent resistivity is due to thermodynamical fluctuations originating from the spin-disorder, which, according to our calculations, can be described reasonably well via the disordered local moments model. Results based on this model agree reasonably well with the measured values of spin-disorder induced resistivity. Finally, we will also discuss the pressure-dependence of the Curie temperature and the spin-disorder part of the resistivity and compare our estimates with available experimental data.

Date: Monday, Jan 17, 2011 16:00

Location: Seminar room 138C (TU Freihaus 9. Stock, **gelb**)
A-1040 Wien, Wiedner Hauptstraße 8-10