INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

Prof. Peter Entel
Physics Department and Center for Nanointegration CENIDE
University Duisburg-Essen, Germany

Monday, January 12, 4 p.m.
ICAMS Seminar room UHW 1102

High performance computing of magnetic nanoparticles

The petaflop/s landmark by the Roadrunner project at the Los Alamos National Laboratory marks the preliminary peak of an impressive development in the high performance computing sector. Also state-of-the- art supercomputers as the IBM Blue Gen/P at the Forschungszentrum Jülich allow nowadays to investigate large systems of the order of 1000 and more spin-polarized transition metals by means of density functional theory. I will present two applications where large-scale ab initio calculations contribute to the understanding of key properties emerging from a close interrelation between structure and magnetism like the size dependent evolution of equilibrium structural motifs in elementary iron and binary Fe-Pt and Co-Pt transition metal nanoparticles. In particular, the latter two materials may play an increasingly important role in future magnetic storage devices.