The ICAMS Seminar presents

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

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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.

For more information contact Dr. Rebecca Janisch, rebecca.janisch@rub.de