CFEL SCIENCE

# SEMINAR

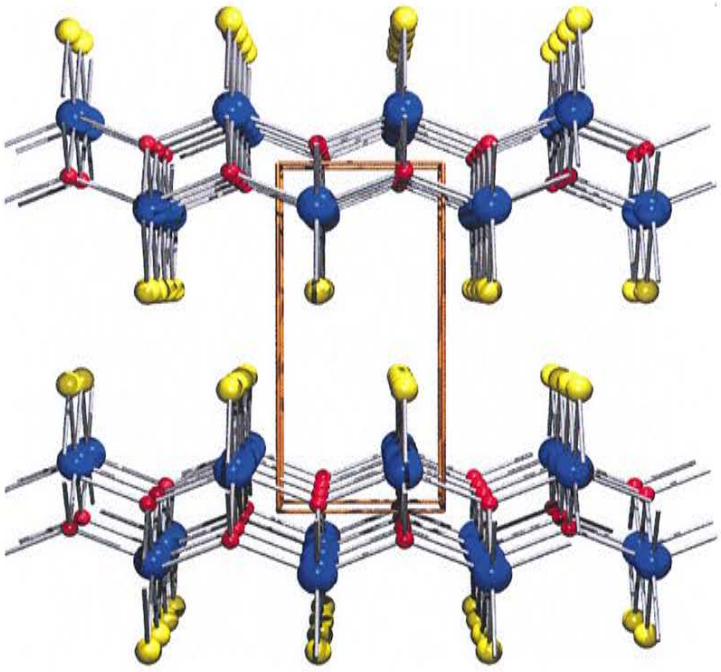
September 22nd, 2010, 10.00 a.m. – DESY Bldg. 49, Room 108


## Harald Jeschke

**Goethe-Universität Frankfurt, Institut für Theoretische Physik**


## Explaining and predicting phase transitions using tight binding and ab initio molecular dynamics


We employ Car Parrinello molecular dynamics simulations at constant pressure in order to study pressure induced phase transitions. In the low-dimensional Mott insulator TiOCl, we find two consecutive phase transitions, first to a dimerized metallic phase and at higher pressure to a uniform metallic phase. In the iron pnictide superconductor family AFe2As2 (A=Ca, Sr, Ba) under pressure, we find that the structural phase transition from orthorhombic to tetragonal symmetry is always accompanied by a magnetic phase transition in all the compounds while the nature of the transitions is different for the three systems. Our calculations explain the origin of the existence of a collapsed tetragonal phase in CaFe2As2 and its absence in BaFe2As2. In an investigation of the physical mechanisms for damage formation in graphite induced by femtosecond laser pulses we perform tight binding molecular dynamics simulations on time-dependent potential energy surfaces. Our predictions of a preablation mechanism were confirmed by experiment.

**Host: Robin Santra, CFEL Theory Group**