TECHNISCHE UNIVERSITÄT CHEMNITZ

# PHYSIKALISCHES KOLLOQUIUM

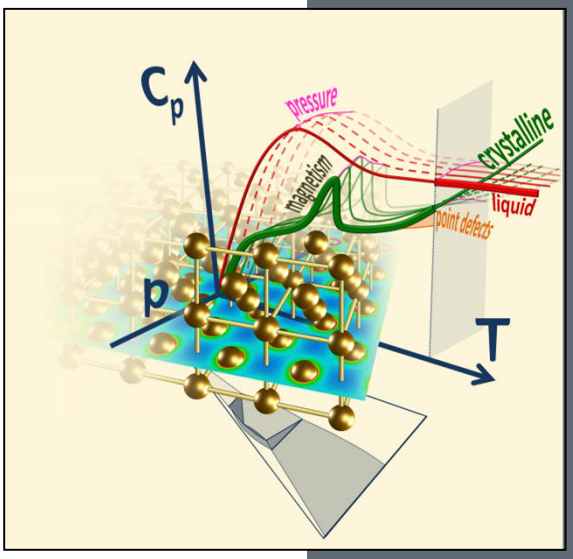
Mittwoch, 16.04.2014, um **16:00 Uhr**

Ort: Reichenhainer Str. 90; Neues Hörsaalgebäude, Raum: 2/N013


## Dr. Tilmann Hickel

*Max-Planck-Institut für Eisenforschung, Düsseldorf*


## *Understanding complex materials at finite temperatures by ab inito methods*




Fully parameter-free ab initio methods based on density functional theory are steadily gaining popularity. Their atomistic view on physical processes and the access to chemical trends are attractive for a knowledge-driven development of novel electronic, biological or engineering materials. However, the apparent restriction of the method to ground state properties is a severe challenge for the understanding and prediction of many materials properties, as, e.g., heat capacities and phase diagrams, for which finite temperature effects are decisive.
Within this talk key ideas how to go beyond this limitation will be presented, with the focus on the new physical insight that can be gained in this way.
Examples include the discovery of universal quantum corrections of magnetic excitations, of large anharmonic contributions to point-defect formation energies as well as the critical and unexpected role of non-adiabatic coupling effects stabilizing certain phases. Some of the findings, obtained with a hitherto not achievable accuracy, helped to resolve long-standing physical questions. At the same time the methods provide access to new routes in materials design as will be demonstrated for the deformation behavior of modern high-strength steels or the nature of phase transitions in magnetic shape-memory alloys.

Alle Zuhörer sind ab 15:45 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt Dr. Sebastian Fähler, Tel.: 0351 4659 588