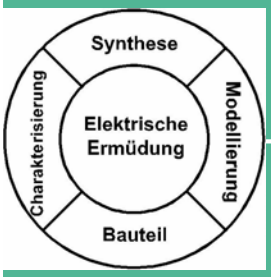

Sonderforschungsbereich 595

Elektrische Ermüdung in Funktionswerkstoffen

TECHNISCHE UNIVERSITÄT DARMSTADT

Sonderkolloquium im WINTERSEMESTER 2009/2010

24.11.
2009

PD Dr. Volker Eyert

Center for Electronic Correlations and Magnetism
Institute for Physics, University of Augsburg

From Frustration to Application: All-Electron DFT Calculations in Materials Science

The delafossite class of materials offers a large variety of phenomena resulting from a broad spectrum of chemical compositions crystallizing in a common structure. Physical properties are strongly influenced by the low dimensionality and include exceptional electronic conductivities and exciting magnetic ordering effects. This has attracted much interest in these materials for reasons of both fundamental interests and applications. In my talk I will discuss some of the delafossite materials from the point of view of state-of-the-art DFT calculations.

The calculations are based on a new all-electron full-potential spherical wave based code, which has proven to be both very accurate and efficient. The basic ideas of this breakthrough in method development will be also briefly sketched in this talk.

Der Vortrag findet um **15:00** im **CSI** Gebäude,
Lichtwiese, Petersenstr. 32, **Raum 23** statt