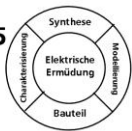


SFB 595



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Sonderforschungsbereich 595 Elektrische Ermüdung in Funktionswerkstoffen



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Kolloquium im
WINTERSEMESTER 2011/2012

**27.10.
2011**

Prof. Igor Kornev

Laboratoire Structures, Propriétés et Modélisation
des Solides, Ecole Central Paris

First-principles effective Hamiltonian based modeling of ferroics

Abstract:

First-principles-based computational approaches have proved to be powerful methods in recent years for understanding ferroic materials. In this talk, a first-principles-based scheme that incorporates ferroelectric, elastic and antiferrodistortive degrees of freedom, as well as magnetic degrees of freedom allowing the computation of finite-temperature properties of ferroics with perovskite structure will be presented. Here I illustrate the efficiency of this computational method to bulk PZT and BiFeO₃ in providing understanding of the fundamental physics and predicting novel phenomena in advance of experimental measurements.

Challenges and opportunities towards the long-sought goal of materials-by-design arising from recent advances in atomic-scale modeling of finite-temperature properties of (multi)ferroics will also be discussed in this talk.

Die Vortrag findet um **16:15 Uhr** im Gebäude der Materialwissenschaften,
Lichtwiese, Petersenstr. 23, Raum 128, statt.