SFB 595 Deutsche Forschungsgemeinschaft DFG

Sonderforschungsbereich 595

Elektrische Ermüdung in Funktionswerkstoffen

TECHNISCHE UNIVERSITÄT DARMSTADT

Kolloquium im
WINTERSEMESTER 2011/2012

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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.