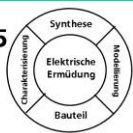


SFB 595



Deutsche
Forschungsgemeinschaft

DFG

Sonderforschungsbereich 595 Elektrische Ermüdung in Funktionswerkstoffen



TECHNISCHE
UNIVERSITÄT
DARMSTADT

*Kolloquium im
WINTERSEMESTER 2011 / 2012*

**10.11.
2011**

Prof. Massimiliano Stengel
Institut de Ciencia de Materials de Barcelona
(CSIC), Bellaterra, Spain

First-principles nanoelectronics: Oxide thin-film devices by design

With the continued demand for portability and speed in consumer electronics, there is an increasing motivation to consider alternative paradigms to conventional silicon-based semiconductor designs. Heterostructures based on ferroelectric and/or magnetic complex oxide thin films are a very promising route to the realization of ultra-compact and ultra-fast electronic devices, due to the high tunability and multiple functionality of these materials. Such properties, however, are often dramatically modified at the nanoscale, and the physics of this size reduction is often poorly understood.

First-principles electronic structure methods are in principle a very powerful tool to addressing these key questions with high predictive power. However, a proper treatment of an applied external bias potential in density-functional theory, which is mandatory for the simulation of realistic devices, has been a very challenging task until very recently. In the first part of this talk, I will show how our recent methodological advances in finite-field techniques have overcome this obstacle [1,2], thus providing full control over the electrical boundary conditions in periodic insulators and capacitors. In the second part of this talk I will present some recent applications of these methods to a number of important technological problems, including the dielectric "dead layer" in paraelectric [3] and ferroelectric [4] thin-film capacitors, and its impact on the band offset at the metal/ferroelectric interface [5,6].

[1] M. Stengel, N. A. Spaldin and D. Vanderbilt, *Nature Physics* 5, 304 (2009).

[2] M. Stengel and N. A. Spaldin, *Phys. Rev. B* 75, 205121 (2007).

[3] M. Stengel and N. A. Spaldin, *Nature* 443, 679 (2006).

[4] M. Stengel, D. Vanderbilt and N. A. Spaldin, *Nature Materials* 8, 392 (2009).

[5] M. Stengel, D. Vanderbilt, and N. A. Spaldin *Phys. Rev. B* 80, 224110 (2009).

[6] M. Stengel, P. Aguado-Puente, N. A. Spaldin, and J. Junquera *Phys. Rev. B* 83, 235112 (2011)

Die Vortrag findet um **16:15 Uhr** im Gebäude der Materialwissenschaften,
Lichtwiese, Petersenstr. 23, **Raum 77**, statt.