

Subject: MSD Colloquium, Stengel, Thurs, 9/13, 11am, 200, Auditorium
From: Suzanne Kokosz <kokosz@anl.gov>
Date: Thu, 30 Aug 2007 14:42:13 -0500
To: Materials Science Division <msd@anl.gov>

MATERIALS SCIENCE COLLOQUIUM

SPEAKER: DR. MASSIMILANO STENDEL
University of California, Santa Barbara

TITLE: ³First-principles modeling of field effects at metal-oxide heterojunctions²

DATE: Thursday, September 13, 2007

TIME: 11:00 a.m.

PLACE: Building 200, Auditorium

HOST: Serge Nakhmanson

Refreshments will be available at 10:45 a.m.

Abstract:

When the thickness of an oxide film is reduced to few unit cells, its dielectric properties (which are relevant, e.g., for nonvolatile ferroelectric memories and as gate oxides in MOSFET transistors) tend to deviate from those predicted by macroscopic models, and are dominated on one side by interfacial chemistry and electrostatics, and on the other side by quantum size effects within the film. One particularly important issue is the ³dielectric dead layer², which plagues the performance of thin-film perovskite capacitors by substantially reducing the effective permittivity (k) of the active high- k material. The microscopic origins of this reduced permittivity, and in particular whether it stems from defects or from the fundamental properties of a metal/insulator interface, are not well understood.

To address this problem from first principles, we will first show how the macroscopic polarization (and the coupling to an external field) can be rigorously defined for a periodic metal-insulator heterostructure [1], by using techniques and ideas borrowed from Wannierfunction theory [2]. We will then demonstrate our new method by calculating the dielectric properties of realistic SrRuO₃/SrTiO₃/SrRuO₃ nanocapacitors [3]. Building on these ideas, we will finally present two closely related applications of our finite-field method in the context of i) monodomain ferroelectricity, and ii) magnetoelectric effects at the interface between a dielectric and a metallic ferromagnet.

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

[2] M. Stengel and N. A. Spaldin, Phys. Rev. B 73, 075121 (2006).

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

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