

Subject: MATERIALS SCIENCE COLLOQUIUM, Professor Javier Junquera, Universidad de Cantabria, Spain, First-principles modeling of ferroelectric oxide nanostructures, Thursday, March 6, 2008, 11:00 a.m., Building 212, Room A-157, Serge Nakhmanson
From: Marlene Metz <metz@anl.gov>
Date: Fri, 22 Feb 2008 08:55:06 -0600
To: msd@anl.gov

MATERIALS SCIENCE COLLOQUIUM

SPEAKER: Professor Javier Junquera
Universidad de Cantabria, Spain

TITLE: "First-principles modeling of ferroelectric oxide nanostructures"

DATE: Thursday, March 6, 2008

TIME: 11:00 a.m.

PLACE: Building 212, Room A-157

HOST: Serge Nakhmanson

Refreshments will be available at 10:45 a.m

Abstract: The field of ferroelectric thin films is at a momentous stage. Recent breakthroughs in the synthesis of complex oxides have recently brought the field to an entirely new level, allowing complex artificial oxide structures to be realized with an atomic-level precision [1, 2]. Not only can high-quality ultrathin oxide films now be grown directly on silicon[3] but, more generally, various type of functional oxides such as ferroelectrics, high-temperature superconductors and magnetic oxides can be combined at the nanoscale, thus offering tremendous new possibilities for artificial multifunctional materials and devices [4]. Hand by hand with these experimental improvements, within the last decade, first-principles simulations on ABO₃ oxides have expanded spectacularly. The steady growth of computing power and the development of methods based on density functional theory (DFT) nowadays permit accurate first-principles atomistic simulations of larger and more realistic systems, overlapping in size and complexity with those that can be grown experimentally.

Despite all the progress made in the last few years, there exists still a conundrum on the phase diagrams of epitaxial ferroelectric thin films, as a function of thickness, composition, temperature and strain [5, 6]. The main reason for the poor understanding of some of the size-effects on ferroelectricity is the vast amount of different effects that compete and might modify the delicate balance between the long-range dipole-dipole electrostatic interactions and the short-range forces, whose subtle equilibrium is known to be at the origin of the ferroelectric instability. Particularly important is the influence of the mechanical and electrical boundary conditions. On the one hand, the strain effects imposed by the substrate might stabilize phases that are not the most stable at the bulk level [7, 8]. On the other hand, unless a perfect screening is provided by free charges from the electrodes or from adsorbates [9], the residual depolarizing field tends to suppress the later [10]. In the case of imperfect screening two typical mechanisms are observed to reduce the electrostatic energy associated with the depolarizing field: (i) the break down of the system into 180° stripe domains [11–13] (recently predicted to exhibit a domain-of-closure structure [14, 15]) and (ii) a uniform progressive reduction of the polarization [16]. In this colloquium, I would like to summarize the most recent advances in the first-principles study of ferroelectric oxide epitaxial thin films. I shall discuss in detail the key roles of mechanical and electrical boundary conditions, providing the basic background for a simple and intuitive understanding of the evolution of the ferroelectric properties in many nanostructures.

[1] Ch. Ahn, J. Mannhart, and J.-M. Triscone, *Nature* 424, 1015 (2003). [2] Ch. Ahn, J.-M. Triscone, and K. M. Rabe, *Science* 303, 488 (2004). [3] R. A. McKee, F. J. Walker, and M. F. Chisholm, *Phys. Rev. Lett.* 81, 3014 (1998). [4] G. Rijnders and D. H. A. Blank, *Nature* 433, 369 (2005). [5] M. Dawber, K. M. Rabe, and J. F. Scott, *Rev. Mod. Phys.* 77, 1083 (2005). [6] Ph. Ghosez and J. Junquera, *First-Principles Modeling of Ferroelectric Oxide Nanostructures*, in *Handbook of theoretical and computational nanotechnology*, edited by M. Rieth and W. Schommers (American Scientific Publishers, Stevenson Ranch, CA, 2006), vol. 9, pp. 623–728, pre-print available at <http://xxx.lanl.gov/abs/cond-mat/0605299>. [7] O. Dieguez, S. Tinte, A. Antons, C. Bungaro, J. B. Neaton, K. M. Rabe, and D. Vanderbilt, *Phys. Rev. B* 69, 212101 (2004). [8] H. N. Lee, H. M. Christen, M. F. Chisholm, C. M. Rouleau, and D. H. Lowndes, *Nature* 433, 395 (2005). [9] D. D. Fong, A. M. Kolpak, J. A. Eastman, S. K. Streiffer, P. H. Fuoss, G. B. Stephenson, C. Thompson, D. M. Kim, K. J. Choi, C. B. Eom, I. Grinberg, and A. M. Rappe, *Phys. Rev. Lett.* 96, 127601 (2006). [10] J. Junquera and Ph. Ghosez, *Nature* 422, 506 (2003). [11] S. K. Streiffer, J. A. Eastman, D. D. Fong, C. Thompson, A. Munkholm, M. V. R. Murty, O. Auciello, G. R. Bai, and G. B. Stephenson, *Phys. Rev. Lett.* 89, 067601 (2002). [12] D. D. Fong, G. B. Stephenson, S. K. Streiffer, J. A. Eastman, O. Auciello, P. H. Fuoss, and C. Thompson, *Science* 304, 1650 (2004). [13] V. Nagarajan, J. Junquera, J. Q. He, C. L. Jia, K. Lee, Y. K. Kim, T. Zhao, Ph. Ghosez, K. M. Rabe, S. Baik, R. Waser, and R. Ramesh, *J. Appl. Phys.* 100, 1 (2006). [14] S. Prosandeev and L. Bellaiche, *Phys. Rev. B* 75, 172109 (2007). [15] P. Aguado-Puente and J. Junquera, <http://arxiv.org/abs/0710.1515>. [16] C. Lichtensteiger, J.-M. Triscone, J. Junquera, and Ph. Ghosez, *Phys. Rev. Lett.* 94, 047603 (2005).

labcast-MSD mailing list

labcast-MSD@lists.anl.gov

<https://lists.anl.gov/mailman/listinfo/labcast-msd>