MATERIALS SCIENCE COLLOQUIUM

SPEAKER: Serge M. Nakhmanson
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TITLE: Understanding, Enhancing and Fine-tuning
Polar Properties in Multicomponent Perovskite Materials

DATE: Thursday, June 28, 2007

TIME: 11:00 a.m.

PLACE: Building 200, Auditorium

HOST: Maria Iavarone

**********NOTE BUILDING CHANGE**********

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

Abstract:

Modern epitaxial thin-film techniques make it possible to synthesize
artificial multicomponent perovskite-oxide superlattices (SLs) with
interfaces that are atomically flat and compositionally abrupt. The behavior
of such systems is dominated by strong interactions between individual SL
layers, high levels of epitaxial strain and symmetry lowering relative to
the bulk. All of these factors can be manipulated in order to enhance or
custom-tailor the useful polar properties ---such as polarization and
piezoelectric response --- for a wide variety of technological applications.
First-principles computational techniques are a tool of choice to help us
understand how the strain, symmetry (including the presence of electrodes)
and composition of these complex systems influence their polar properties.
Unfortunately, the computational costs associated with such simulations
quickly become prohibitive, which often makes it impossible to answer
various interesting questions, like, e.g., which particular SL layer
arrangement results in the best possible polar properties? Here we show how
first-principles calculations combined with a simple model for SL
polarization and a genetic-algorithm optimization allow us to find an answer
to the question mentioned above and, among other things, to predictively
identify the most polar perovskite-oxide SLs that can be grown on currently
available substrates.