

2008 Workshop on Fundamental Physics of Ferroelectrics
February 10 - 13, 2008
Woodlands Hotel, Williamsburg, Virginia

PROGRAM

Registration and Reception:	<i>Cascades Foyer</i>
Lectures:	<i>Cascades Room</i>
Poster Sessions:	<i>Oak Room</i>

Sunday 10 February 2008

5:00	- Registration and Welcoming Reception - (2 hours)
7:00	- Dinner - Oak Room
9-11	- Informal discussions at Huzzah -

Monday 11 February 2008

- 7:30 - 10:00 - **Registration** -
- 8:25 **Welcome/Announcements: Cohen**
- Multiferroics: Vanderbilt - Session Chair**
- 8:30 Harris (I) Order parameters and phase diagrams of multiferroics
- 9:00 Scott (I) Smorgasbord of multiferroics
- 9:30 Kornev Finite-temperature properties of multiferroic BiFeO₃ from first principles
- 9:50 Mardana Magneto-electric effects in ferromagnetic cobalt/ferroelectric copolymer multi-layer films
- 10:10 Fennie Ferroelectrically induced weak-ferromagnetism by design
- 10:30 - **Coffee Break** - (1/2 hour)
- Surfaces/Interfaces: Rabe - Session Chair**
- 11:00 Rappe Interplay of bulk ferroelectric polarization and the oxide surface environment
- 11:20 Levy A ferroelectric oxide directly on silicon
- 11:40 Levchenko The influence of ferroelectric polarization on the equilibrium stoichiometry of ferroelectric surfaces
- 12:00 - **Lunch** - Dogwood Room (1 1/2 hours)
- Thin Films I: Junquera - Session Chair**
- 1:30 Triscone (I) Tailored and improper ferroelectricity in PbTiO₃/SrTiO₃ superlattices: I. Experimental results
- 1:55 Bousquet (I) Tailored and improper ferroelectricity in PbTiO₃/SrTiO₃ superlattices: II. Theoretical results
- 2:20 Tenne Size and strain effect on phase transitions in ultrathin BaTiO₃ films and BaTiO₃/SrTiO₃ superlattices studied by ultraviolet Raman spectroscopy
- 2:40 Uesu (I) Peculiar structural and dielectric properties of relaxor/FE superlattice films fabricated on the single lattice scale
- 3:10 **Posters M1-M17** - Oak Room (2 hours)
- Relaxors: Colla - Session Chair**
- 5:10 Vakhrushev(I) Formation and temperature evolution of the polar nanoregions in relaxors
- 5:40 Xu (I) Phase instability induced by polar nanoregions in a relaxor ferroelectric
- 6:10 Hlinka (I) Soft mode dispersion and "waterfall" phenomenon in relaxors revisited
- 6:40 Schmidt Electric-field poling effect and nanotwins in Pb(Mg_{1/3}Nb_{2/3})_{0.70}TiO₃
- 7:00 End
- 7:00 - **Dinner** - Dogwood Room
- 9-11 - **Informal discussions at Huzzah** -

Tuesday 12 February 2008

Defects, Domains, and Nanostructures: Scott - Session Chair

- 8:30 Burton (I) Correlations between the cation and anion-components of Schottky defects in HfO_2 , $\text{Pb}(\text{Sc}_{1/2}, \text{Nb}_{1/2})\text{O}_3$, and NaCl
- 9:00 Salje (I) Surface nucleation and lateral movement of ferroelastic domain walls
- 9:30 Maksymovych Direct imaging of spatial and energy distribution of nucleation centers in ferroelectric materials
- 9:50 Davies Nanoscale modulations in Li-based perovskites
- 10:10 Roytburd Theory and modeling of domain evolution in graded multilayers and films

10:30 - **Coffee Break** - (1/2 hour)

Thin Films II: Triscone - Session Chair

- 11:00 Junquera (I) Ferromagnetic-like closure domains in ferroelectric ultrathin films
- 11:30 Nakhmanson Critical thickness for ferroelectricity in ultrathin perovskite films with inequivalent electrodes

12:00 - **Lunch** - Dogwood Room (1 1/2 hours)

Phase Transitions in Perovskites I: Yacoby - Session Chair

- 1:30 Takeuchi (I) Combinatorial discovery of a ferroelectric-antiferroelectric morphotropic phase boundary in doped BiFeO_3 films
- 2:00 Rabe Competing lattice instabilities and structural transitions in complex oxides from first principles
- 2:30 Kamba Ferroelectricity in SrTiO_3 and EuTiO_3 strained thin films: Polar phonon properties
- 3:00 Ponomareva High-frequency dielectric response of paraelectric BaTiO_3

3:20 **Posters T1-T17** - Oak Room (2 hours)

New Materials and Design: Resta - Session Chair

- 5:20 Cohen Theoretical and experimental studies for new transducer materials
- 5:50 Bellaiche Properties of ferroelectrics, ferromagnetics, and multiferroics from atomistic simulations

6:10 End

7:00 - **Banquet at James Shields Tavern** -

9-11 - **Gambols at James Shields Tavern** -

Wednesday 13 February 2008

Phase Transitions in Perovskites II: Bellaiche - Session Chair

- 8:30 Yacoby (I) Ti off-center displacements and the oxygen isotope induced phase transition in SrTiO₃
- 9:00 Bussmann-Holder Complexity in the phase diagram of perovskite ferroelectrics
- 9:20 Bokov Experimental study of the relationship between nanoscale structure and dipole dynamics in relaxor ferroelectrics
- 9:40 Taniguchi Ferroelectric phase transition and soft mode in CdTiO₃ studied by Raman scattering ~ A quest for ideal quantum critical point in soft mode system ~
- 10:00 Yao First-principles study of polarization saturation in ferroelectric perovskites
- 10:20 Yamanaka Pressure dependence of electron density distribution of KNbO₃, BaTiO₃, and PbTiO₃ by maximum entropy method using single crystal diffraction

10:40 - **Break** - (1/2 hour)

Theoretical Methods: Cohen - Session Chair

- 11:10 Vanderbilt Nonlinear dielectric response via calculations at fixed electric displacement field
- 11:40 Krakauer Finite-size correction in many-body electronic structure calculations: Post-processing corrections using density functional theory with finite-size exchange and correlation
- 12:10 Prosandeev Control of vortices by homogeneous fields in asymmetric ferroelectric and ferromagnetic rings: A unifying theoretical approach

12:30 Close

12:30 - **Lunch** - Dogwood Room (1 1/2 hours)

Poster Session I: Monday 11 February 2008

- M1 Ahart, M. Pressure-temperature effects on diffuse scattering in relaxor ferroelectrics
- M2 Beckman, S. Strained films of PTO and PZT
- M3 Bennett, J. Decreasing the band gap of PbTiO_3 : Ferroelectrics of the future
- M4 Bin-Omran, S. Dependence of polarization on epitaxial strain in ferroelectric ultrathin films from first principles
- M5 Coh, S. Stability and lattice dynamics of SiO_2 cristobalite
- M6 Colla, E. Glasslike aging of the polarized relaxors
- M7 Cooper, V. Polarization of ferroelectric perovskite superlattices from first principles
- M8 Ducharme, S. Apparatus for pyroelectric scanning microscopy
- M9 Ducharme, S. Spectroscopic and density functional theory studies of vinylidene fluoride oligomers
- M10 Eglitis, R. Ab initio calculations of BaTiO_3 , PbTiO_3 , and SrTiO_3 (001) and (011) surface structures
- M11 Fonari, M. GGA+U calculation of the dielectric response of perovskite oxides
- M12 Ganesh, P. Search for new high performance piezoelectrics
- M13 Ishii, F. First-principles study of electric polarization in multiferroics with non-collinear magnetic structures
- M14 Janolin, P.-E. Thickness-controlled structure of ferroelectric thin films
- M15 Kagimura, R. First-principles investigations of elastic properties, energetics and Pb anti-site defects in Pb-based perovskites
- M16 Katiyar, R. Phase transition studies in multiferroic BiFeO_3 thin films using Raman spectroscopy
- M17 Kuznetsov, A. Probability density approach for ferroelectric ordering

Poster Session II: Tuesday 12 February 2008

- T1 Lee, J.H. Ferroelectric order in oxide superlattices
- T2 Lisenkov, S. Domains switching in epitaxial BaTiO₃/SrTiO₃ superlattices from first principles
- T3 Lokshin, K. Effect of Ba substitution for Pb in the structure of PZT, Pb_{1-x}Ba_xZr_{0.65}Ti_{0.35}O₃
- T4 Louis, L. Investigation of BaTiO₃ nanowires and nanocomposites from first principles
- T5 Matsuura, M. Neutron diffuse scattering study of the relaxor ferroelectric (1-x)Pb(Mg_{1/3}Nb_{2/3})O₃-xPbTiO₃ near the MPB (x=0.34)
- T6 Mitchell, D. Local structure of complex phases of NaNbO₃ by neutron PDF
- T7 Moriwaki, H. First-principles study on the anisotropic behavior of permittivity of tetragonal-phase BaTiO₃
- T8 Nishimatsu, T. Molecular dynamics simulations of hysteresis loop for BaTiO₃ ferroelectric thin-film capacitors using the feram code
- T9 Ohwada, K. Intrinsic ferroelectric instability in Pb(In_{1/2}Nb_{1/2})O₃ revealed by changing B-site randomness: Inelastic x-ray scattering study
- T10 Palova, L. Ideal nanocheckerboard BiFe_{0.5}Mn_{0.5}O₃ from first principles
- T11 Pechkis, D.L. First principles calculations of nuclear magnetic resonance (NMR) chemical shielding of ¹⁷O in PZT
- T12 Qi, T. Structure and energetics of Bi(Zn,Ti)O₃
- T13 Soon, H.P. "Dirty" classical to quantum crossover in ferroelectricity
- T14 Tsukada, S. Brillouin scattering of lead titanate grown by a floating-zone technique
- T15 Tsukada, S. Dynamical properties of polar nanoregions of relaxor ferroelectric Pb(Ni_{1/3}Nb_{2/3})O₃-0.29PbTiO₃
- T16 Wakimoto, S. Linear relation between electric polarization and magnetic chirality in the commensurate phase of RMn₂O₅ (R=Ho, Er)
- T17 Yokota, H. Critical phenomenon observed in quantum relaxor KTaO₃ doped with Li