2006 Workshop on Fundamental Physics of Ferroelectrics
February 12–15, 2006
Woodlands Hotel, Williamsburg, Virginia

Program

SUNDAY, FEBRUARY 12, 2006

5:00 – 7:00 PM	Registration and Welcoming Reception	*Cascades Foyer*
7:00 – 9:00	Dinner	*Oak Room*

MONDAY, FEBRUARY 13, 2006

7:45 – 8:25 AM	Registration	*Outside Cascades Room*
8:25 – 8:30	Welcome - Cohen	*Cascades Room*
Session I. Theory I (Chair – D. Vanderbilt)		
8:30 – 8:50	L. Bellaiche	Unusual phenomena in ferroelectrics
8:50 – 9:10	A. Rappe	Relating first principles calculations, crystal chemistry, and properties of ferroelectric perovskites
9:10 – 9:30	H. Krakauer	First principles studies of the local structure of $Pb(Zr_{1-x}Ti_x)O_3$ (PZT)
9:30 – 9:50	D. Singh	Electronic structure and bond competition in the polar magnet $PbVO_3$
9:50 – 10:10	D. Bilc	Interplay between electronic structure and cage effects in niobate perovskites: $(K,Li)NbO_3$ and $PbMg_{1/3}Nb_{2/3}O_3$
10:10 – 10:30	R. Cohen	Origin of large response in high electromechanical coupling transducer materials
10:30 – 11:00	**COFFEE BREAK**	
Session II. Theory II (Chair – H. Krakauer)		
11:00 – 11:30	B. Burton (invited)	First principles based simulations of PSN and PMN
11:30 – 11:50	D. Vanderbilt	Finite electric fields and non-linear responses in ferroelectrics
11:50 – 12:10 PM	K. Rabe	Predicting polarization enhancement in multicomponent ferroelectric superlattices
12:10 – 12:30	I. Naumov	An efficient approach and its underlying mechanism of switching vortex moment in ferroelectric nanoparticles
12:30 – 1:40 PM	**LUNCH**	*Dogwood Room*
Session II. Theory II cont. (Chair – B. Burton)		
1:40 – 2:10	R. Resta (invited)	Polarization fluctuations in classical and quantum systems
2:10 – 2:30	W. Al-Saidi	Auxiliary field Quantum Monte Carlo study of atoms and molecules using localized basis sets
Session III. Experiment (Chair – H. Schmidt)		
2:30 – 2:50	P. Davies	Enhanced tetragonality in $PbTiO_3 – Bi(B'B'')O_3$ solid solutions
2:50 – 3:10	T. Egami	Giant dielectric permittivity and magnetocapacitance in $La_{0.875}Sr_{0.125}MnO_3$ single crystals
3:10 – 3:30	G. Malovichko	Radiation defects in complex ferro – and piezoelectric oxides
3:30 – 3:50	N. Dalal	KH_2PO_4(KDP) revisited: some old questions and new results
3:50 – 5:50	**COFFEE BREAK**	**POSTER SESSION I** (Odd numbers) – *Oak Room*
Session IV. Thin Films I (Chair – Y. Yacoby)		
5:50 – 6:20	B. Noheda (invited)	Thin films of lead titanate under tensile strain
6:20 – 6:40	H. Lee	Weak strain-polarization coupling and ferroelectricity in epitaxially strained $PbZr_{0.2}Ti_{0.8}O_3$ (ultra)thin films
6:40 – 7:00	J. Woicik	Strain induced ferroelectric $SrTiO_3$ thin films grown coherently on Si(001): experiment and theory
7:30 – 9:00	**DINNER**	*Dogwood Room*

Poster Sessions

MONDAY, FEBRUARY 13, 2006: Session I (Odd numbers)
TUESDAY, FEBRUARY 14, 2006: Session II (Even numbers)

P1	Muhtar Ahart, Prezemyslaw Dera, Russell J. Hemley, and Ron E. Cohen	*Pressure Induced Phase Transitions in $PbTiO_3$*
P2	Zeyad Alahmed and Huaxiang Fu	*First-Principles determination of chemical potentials and vacancy formation energy in lead titanate and barium titanate*
P3	Emad Almahmoud, Igor Kornev, and Laurent Bellaiche	*Critical Behaviors in $Pb(Zr,Ti)O_3$ Ultrathin films*
P4	Kristopher E. Andersen and C. Stephen Hellberg	*Structural interface and electronic structure of epitaxial $SrTiO_3$ on Si(001)*
P5	Joseph Bennett, Ilya Grinberg, and Andrew M. Rappe	*A First Principles Approach to Modeling $Ba_{(1-x)}Ca_{(x)}ZrO_3$*
P6	Eric Bousquet and Philippe Ghosez	*First-principles study of $(BaTiO_3)_m/(BaO)_n$ multilayers*
P7	Razvan Caracas and Ron E. Cohen	*Searching for ferroelectrics with exotic chemistry*
P8	S. Choudhury, Y. L. Li, and L.Q. Chen	*Phase-field simulations of ferroelectric domain structures and domain switching in ceramics and thin films*
P9	Eric Cockayne	*Influence of oxygen vacancies on the dielectric properties of hafnia*
P10	Eugene V. Colla and Michael B. Weissman	*Remnant polarization as a local probe of the order-disorder in relaxor ferroelectric*
P11	Oswaldo Diéguez and David Vanderbilt	*Constrained polarization study of ferroelectric potassium nitrate*
P12	Alexei Grigoriev, Dal-Hyun Do, Dong Min Kim, Chang-Beom Eom, Paul G. Evans, Bernhard Adams, and Eric M. Dufresne	*Polarization switching dynamics of thin ferroelectric films*
P13	Craig J. Fennie, Karin M. Rabe, and Ram Sheshadri	*Lattice instabilities and polar properties in pyrochlores from first principles*
P14	T. Fukushima and Y. Uesu	*Size-effect of quantum paraelectric $SrTi^{16}O_3$ and $SrTi^{18}O_3$ thin films*
P15	Guido Gerra, A. K. Taganstev, N. Setter, and K. Parlinski	*Ionic polarizability of conductive metal-oxides and critical thickness for ferroelectricity in $BaTiO_3$*
P16	Ilya Grinberg and Andrew M. Rappe	*The origin of T_c nonlinearity in Bi-based ferroelectric perovskite solid solutions*
P17	Holger Hellwig, Alp Sehirlioglu, David A. Payne, and Pengdi Han	*New soft-mode in $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$*
P18	Jirka Hlinka, M. Kempa, J. Kulda, P. Bourges, A. Kania, and J. Petzelt	*Lattice dynamics of ferroelectric $PbTiO_3$ by inelastic neutron scattering*
P19	Stephen Jesse, Brian Rodriguez, Sergei V. Kalinin, and Marine Alexe	*Quantitative mapping of switching behavior by switching spectroscopy piezoresponse force microscopy*
P20	Brian Rodriguez, Stephen Jesse, and Sergei V. Kalinin	*Piezoresponse force microscopy in liquid environment: ultrahigh resolution and novel physics*
P21	Diana Kaynts, Andrew Horvat, Alexander Grabar, Ivan Stoika, and Mikhail Gurzan	*Domain configuration in $Sn_2P_2S_6$ ferroelectrics-semiconductors*
P22	Alexie M. Kolpak, Na Sai, and Andrew M. Rappe	*Using surface chemistry to modify charge passivation in ultrathin ferroelectric films*
P23	Bo-Kuai Lai, I. Ponomareva, I. I. Naumov, I. Kornev, Huaxiang Fu, L. Bellaiche, and G. J. Salamo	*Domain evolution in ferroelectric ultrathin films under external electric field*
P24	C. Laulhé, F. Hippert, J. Kreisel, M. Maglione, A. Simon, J.L. Hazemann, and V. Nassif	*EXAFS study of lead-free relaxor ferroelectric $BaTi_{1-x}Zr_xO_3$*
P25	Shen Li, Craig J. Fennie, and Karin M. Rabe	*Ferroelectricity and multiferroicity in the Dion-Jacobson compounds $ABiNb_2O_7$, A=Cs, (MnCl), from first principles*
P26	Sergey Lisenkov, Laura Walizer, and L. Bellaiche	*Modeling finite temperature properties of $(Ba,Sr)TiO_3$ disordered alloys and $BaTiO_3/SrTiO_3$ superlattices from first principles*
P27	Lydie Louis, I. Ponomareva, I. Kornev, and L. Bellaiche	*Investigation of $BaTiO_3$ nanowires from first principles*
P28	Hiroki Moriwake, Ryusuke Teramoto, Kentaro Tomoda, Kazuyoshi Ogasawara	*First-principles calculations of ferroelectric phase of $CaTiO_3$*

P29	S. M. Nakhmanson, K. M. Rabe, and David Vanderbilt	*Predicting polarization enhancement in multicomponent ferroelectric superlattices*
P30	W.D. Nothwang, K.P. Mohanchandran, J.D. Demaree, J.K. Hirvonen, S.G. Hirsch, C. Hubbard, E. Ngo, M.W. Cole	*Thin film ferroic materials for mitigating harsh vibrational environments*
P31	S. Panigrahi, S. K. Rout and T. BadaPanda	*Spin glass analogy of ABO_3 relaxor ferroelectric: A theoretical model*
P32	D. L. Pechkis, E. J. Walter, and H. Krakauer	*Cluster calculations of nuclear magnetic resonance chemical shielding in solids*
P33	Brian Rodriguez, Stephen Jesse, Sergei V. Kalinin, Jihee Kim and Stephen Ducharme	*Imaging and polarization dynamics in ultrathin ferroelectric PVDF colpolymers by piezoresponse force microscopy*
P34	A.L.Roytburd	*Engineering elastic domain structures in ferroelectric films with enhanced piezo and electric responses*
P35	Young-Han Shin, Ilya Grinberg, I-Wei Chen, and Andrew M. Rappe	*Understanding ferroelectric domain-wall motion: Multi-scale approach*
P36	D. A. Tenne, A. Bruchhausen, A. Fainstein, R. S. Katiyar, A. Cantarero, A. Soukiassian, W. Tian, D. G. Schlom, Y. L. Li, L. Q. Chen, C.-B. Eom, H. P. Sun, X. Q. Pan, and X. X. Xi	*UV Raman study of lattice dynamics and ferroelectric phase transitions in $BaTiO_3/SrTiO_3$ superlattices*
P37	O.P. Thakur and Derek C. Sinclair	*Dielectric, ferroelectric and impedance spectroscopic behaviour of $Ba(Zr,Ti)O_3$ ceramics processed by attrition milling*
P38	S. Tinte, B.P. Burton, Eric Cockayne, and U. V. Waghmare	*First principles based simulation of the ferroelectric to relaxor transition as a function of pressure in $Pb(Sc_{1/2}Nb_{1/2})O_3$*
P39	Xinjie Wang and David Vanderbilt	*First-principles calculation of Born effective charges and dielectric constants in finite electric fields via a Berry-phase approach*
P40	Xifan Wu, Oswaldo Diéguez, Karin M. Rabe, and David Vanderbilt	*Electrostatics of superlattices by first principles*
P41	A. A. Bokov and Z.-G. Ye	*Crossover from critical behavior to double freezing in $(1- x)Pb(Mg_{1/3}Nb_{2/3})O_3 – xPbTiO_3$ relaxors*
P42	Hiroko Yokota, Taeko Oyama, Yoshiaki Uesu, Charlotte Malibert, and Jean-Michel Kiat	*Two-step change of the polar state in Li-doped $KTaO_3$ - Evidence of polar nano-regions*
P43	Alexey T. Zayak, Serge M. Nakhmanson, and Karin M. Rabe	*Revealing the hidden polar character of $CaTiO_3$*

TUESDAY, FEBRUARY 14, 2006

Session V. Relaxors (Chair – R. Vold)		
8:30 – 9:00 AM	R. Blinc (invited)	Line of critical points near the morphotropic phase boundary and the giant electromechanical response in rerroelectric relaxors
9:00 – 9:20	M. Vijayakumar	NMR study of local structure in (1-x)$PbMg_{1/3}Nb_{2/3}O_3$ – x$PbSc_{1/2}Nb_{1/2}O_3$ across the ferroelectric phase transition
9:20 – 9:40	B. Dkhil	Intrinsic and induced strains in lead-based relaxor ferroelectrics
9:40 – 10:00	Z. Ye	Phase transition in ferroelectric relaxors - A comparative study of $Pb(Sc_{1/2}Nb_{1/2})O_3$, $Pb(Zn_{1/3}Nb_{2/3})O_3$ & $Pb(Mg_{1/3}Nb_{2/3})O_3$
10:00 – 10:20	P. M. Gehring	Electric field effects on the structure and polar nanoregions in $PbMg_{1/3}Nb_{2/3}O_3$
10:20 – 10:50	**COFFEE BREAK**	
Session VI. Thin Films II (Chair – K. Rabe)		
10:50 – 11:20	Y. Yacoby (invited)	Ferroelectricity in ultra-thin perovskite films without electrodes
11:20 – 11:40	J.-G. Yoon	Domain dynamics and a fundamental thickness limit of ultra-thin ferroelectric $BaTiO_3$ capacitors
11:40 – 12:10 PM	P. Ghosez (invited)	First-principles modeling of ferroelectric oxide thin films and multilayers
12:10 – 12:30	M. Cole	Design and development of temperature stable, affordable and performance consistent phase shifters for mobile microwave communications applications
12:30 – 1:30 PM	**LUNCH**	*Dogwood Room*
Session VII. Multiferroics and Relaxors (Chair – T. Egami)		
1:30 – 2:00	J. Kreisel (invited)	Raman scattering in multiferroics: $BiFeO_3$ and related systems
2:00 – 2:20	J. Slutsker	Self-assembled multiferroic thin film nanostructures
2:20 – 2:40	M. Weissman	Evidence for the role of small-scale glassiness in cubic relaxors
2:40 – 3:00	J. Toulouse	Temperature evolution of the relaxor dynamics in $Pb(Zn_{1/3}Nb_{2/3})O_3$: A critical Raman analysis and a microscopic model
3:00 – 3:30	G. Xu (invited)	Electric field induced redistribution of polar nano-regions in a relaxor ferroelectric
3:30 – 5:30	**COFFEE BREAK**	**POSTER SESSION II** (Even numbers) – *Oak Room*
Session VIII. Pressure and Fusion (Chair – R. Cohen)		
5:30 – 5:50	A. Bussmann-Holder	Pressure dependence of T_c and formation of polar micro regions in $SrTi^{18}O_3$
5:50 – 6:10	I. Kornev	Ferroelectricity of perovskites under pressure
6:10 – 6:30	S. Putterman	What is the maximum spontaneous polarization that can be achieved in a ferroelectric crystal used as a particle accelerator?
7:30 – 9:00	**BANQUET**	*Kings Arms Tavern*

WEDNESDAY, FEBRUARY 15, 2006

Session IX. Nanostructures and Vacancies (Chair – L. Bellaiche)		
8:30 – 9:00 AM	S.Vakhrushev (invited)	Porous matrices-based ferroelectric and magnetic materials
9:00 – 9:20	I. Ponomareva	Modeling of ferroelectric nanodots and nanowires under different electrical and mechanical boundary conditions
9:20 – 9:40	S. Prosandeev	Controlling the toroidal moment in ferroelectric dots
9:40 – 10:00	P. Wu	First-principles study of oxygen vacancy formation in B-site doped lead zirconate titanate
10:00 – 10:30	**COFFEE BREAK**	
Session X. Domains (Chair – A. Rappe)		
10:30 – 11:00	J. Scott (invited)	Skyrmion emission of nano-domains in ferroelectrics: Theory and experiment
11:00 – 11:20	K. Bowman	Domain orientation and textures of piezoelectric materials
11:20 – 11:40	H. Schmidt	Dielectric anomalies, domain observations, and optical properties in high-Curie-temperature $Pb(In_{1/2}Nb_{1/2})_{1-x}Ti_xO_3$ single crystals
11:40 – 12:00 PM	W. Kleemann	Universal Domain Wall Dynamics in Disordered Ferroic Materials
12:00 – 12:20	A. Tagantsev	Creep and pinning of ferroelectric domain walls: new features
12:20 – 12:30	**CLOSE**	
12:30 – 1:30 PM	**LUNCH**	*Dogwood Room*