PROGRAM

Sunday, January 29, 2012 (ANL Guest House)

5:00-7:00pm: Registration and Welcome Reception

Monday, January 30, 2012 (TCS Conference Center, Bldg. 240)

7:30-8:00am: Registration
8:00-8:05am: Welcome/Announcements (P. B. Littlewood)
8:05-8:10am: In memoriam: R. Blinc (delivered by J. F. Scott)

Session 1: Novel materials: multiferroics (Session Chair: D. J. Singh)
8:15-8:45am: J. F. Scott (invited) - A New Room-Temperature Multiferroic (Ferromagnetic Ferroelectric): Lead iron-tantalate-zirconium-titanate $Pb(Fe,Ta,Zr,Ti)O_3$
8:45-9:05am: B. Dabrowski - Prediction and Realization of Breakthrough Multi-Ferroic Perovskites
9:05-9:35am: S. Kamba (invited) - Infrared studies of strained magnetoelectric thin films of EuO, $SrMnO_3$ and $Ca_3Mn_2O_7$
9:35-10:05am: A. A. Belik (invited) - High-pressure synthesis of new ferroelectric and multiferroic perovskite materials

10:05-10:30am: COFFEE

Session 2: Novel materials: ferroelectrics (Session Chair: D. Vanderbilt)
10:30-11:00am: R. E. Cohen (invited) - Ferroelectricity under applied pressure and applied electric fields
11:00-11:20am: Y. Uesu - Ferroelectric $(PbSnTi)O_3$ thin films synthesized by nucleation-mixture depositions and their structural and dielectric properties
11:20-11:40am: W. Parker - Epitaxial Strain Tunes Polarization and Electronic Band Gap in perovskite $SnTiO_3$

11:40am-1:00pm: LUNCH (ANL Guest House)

Session 3: Surface/interface compensation (Session Chair: J. A. Eastman)
1:00-1:30pm: M. J. Highland (invited) - Polarization of Ultrathin $PbTiO_3$ with Controlled Surface Compensation
1:30-1:50pm: K. Garrity - Ferroelectric Surface Chemistry: a first-principles study of the $PbTiO_3$ surface
1:50-2:10pm: Y. Watanabe - Properties of intrinsic ferroelectric surface in extreme clean limit: Giant 2D conduction on atomically clean surface of stoichiometric $BaTiO_3$ in UHV
2:10-2:30pm: Y.-M. Kim - Interface Mediated Stabilization of Ferroelectric and Non-Polar Phases of $BiFeO_3$

2:30-3:00pm: COFFEE

Session 4: Topological defects and domains (Session Chair: P. G. Evans)
3:00-3:30pm: L. Bellaiche (invited) - Binding of Electric Vortices with Electric Antivortices in Ferroelectrics and Multiferroics
3:30-4:00pm: S. Kalinin (invited) - Static and dynamics conductance of topological defects in ferroelectrics
4:00-4:20pm: C. Dubourdieu - Study of ferroelectricity in tetragonal $BaTiO_3$ epitaxial films grown on $SrTiO_3$-buffered Si(001) - Can this system exhibit negative capacitance?

4:20-4:40pm: MINI-BREAK

4:40-5:00pm: D. Su - Origin of 90° Domain Wall Pinning in $Pb(Zr_{0.2}Ti_{0.8})O_3$ Heteroepitaxial Thin Films
5:00-5:20pm: Q. Zhang - Domain Wall Dynamics of Ferroelectric Ultrathin Films
5:20-5:40pm: W. Wu - Conduction of topologically-protected charged ferroelectric domain walls
5:40-6:00pm: M. V. Holt – Elastic Relaxation and Local Strain in $BiFeO_3$ Nanostructures

7:00pm DINNER (Maggiano's Little Italy, Oak Brook, IL)

Tuesday, January 31, 2012 (TCS Conference Center, Bldg. 240)

Session 5: **Superlattices (Session Chair: S. M. Nakhmanson)**

8:00-8:30am: P. G. Evans (invited) - Nanosecond Dynamics in Ferroelectric/Dielectric Superlattices

8:30-8:50am: M. Dawber - New $PbTiO_3$ based superlattices with exceptional properties

8:50-9:20am: J. Junquera (invited) - Highly-confined spin-polarized two-dimensional electron gas in $SrTiO_3/SrRuO_3$ superlattices

9:20-9:50am: COFFEE

Session 6: **Phase Transitions (Session Chair: L. Bellaiche)**

9:50-10:10am: A. R. Damodaran - Phase Evolution and Stabilization in Highly-Strained Epitaxial $BiFeO_3$ Films: Implications for Enhanced Electromechanical Response

10:10-10:30am: S. Prosandeev - Novel Properties in $BiFeO_3$ Films

10:30-10:50am: A. Roytburd - Stability and Field Induced Response of Heterophase Nanostructures in Constrained Ferroelectrics and Ferroelastics

10:50-11:10am: Z.-G. Ye - Tricritical Points and Related Properties of $Pb(Zr_{1-x}Ti_x)O_3$ Single Crystals

11:10-11:30am: A. Bussmann-Holder - Tuning the structural instability of $SrTiO_3$ by Eu doping: the phase diagram of $Sr_{1-x}Eu_xTiO_3$

11:30am-1:00pm: LUNCH (ANL Guest House)

Session 7: **Relaxors (Session Chair: R. E. Cohen)**

1:00-1:30pm: A. M. Rappe (invited) - Molecular Dynamics Study of Dielectric Response in a Relaxor Ferroelectric

1:30-1:50pm: C. Stock - Magnetic and ferroelectric relaxor properties in $PbFe_{1/2}Nb_{1/2}O_3$

1:50-2:10pm: S. Vakhrushev - Diffuse scattering in perovskites

2:10-2:40pm: P. M. Gehring (invited) - Anisotropic Acoustic Lattice Dynamics in $PbMg_{1/3}Nb_{2/3}O_3$

2:40-3:00pm: COFFEE

Session 8: **Flexoelectricity (Session Chair: J. Junquera)**

3:00-3:20pm: D. Vanderbilt - First-principles theory of flexoelectricity

3:20-3:40pm: A. Tagantsev - Flexoelectric effect in finite samples

3:40-4:00pm: I. Naumov - Flexoelectric effect in 2D sp^2-bonded crystals

4:00-6:00pm: **POSTERS (TCS Conference Center, Bldg. 240)**

Wednesday, February 1, 2012 (TCS Conference Center, Bldg. 240)

Session 9:	**Modeling (Session Chair: K. M. Rabe)**
8:00-8:30am:	R. Resta (invited) - Dynamical matrix in magnetoelectrics
8:30-8:50am:	N. Benedek - Coexistence of ferroelectricity and octahedral rotations in ABX_3 perovskites
8:50-9:10am:	H. Moriwake – Structural analysis of ferroelectric phase of $CdTiO_3$ from first-principles calcuations
9:10-9:30am:	J. Hong - Spin-phonon coupling effects in transition-metal perovskites: a DFT+U and hybrid-functional study
9:30-9:50am:	E. Walter - First-principles calc of Sc NMR parameters in $Pb(Sc_{2/3}W_{1/3})O_3$
9:50-10:10am:	J. Wojdel - All-atom ab-initio models for perovskite ferroelectrics and lattice mode interactions in $PbTiO_3$
10:10-10:40am:	COFFEE
Session 10:	**Techniques (Session Chair: M. J. Highland)**
10:40-11:00am:	N Barrett - Full field electron spectromicroscopy of ferroelectric materials
11:00-11:20am:	J. W. Freeland - Structural Control of Magnetic Anisotropy in a Multiferroic $EuTiO_3$ Thin Film
11:20-11:40am:	Y. Li - Ultrafast optical manipulation of the ferroelectric order in multiferroic bismuth ferrite
11:40-12:00pm:	A. Lindenberg - Ultrafast terahertz and x-ray probes of ferroelectric structural and electronic dynamics

12:00pm: LUNCH (ANL Guest House) and adjourn

Poster Session, Tuesday, Jan 31, 4-6pm (TCS Conference Center, Bldg. 240)

	Author(s)	Title	Subject
PS01	M.C. Ehmke, J.E. Blendell, K.J. Bowman	The Influence of Phase Coexistence and Ferroelastic Domain Texture on the Performance in $Ba(Zr_{0.2}Ti_{0.8})O_{3-x}(Ba_{0.7}Ca_{0.3})TiO_3$ Piezoceramics	Domains
PS02	J. Karthik, A. R. Damodaran, L. W. Martin	Effect of 90° domain walls on the dielectric and pyroelectric susceptibilities of epitaxial ferroelectric thin films	Domains
PS03	T. Nishimatsu, K. Aoyagi, T. Kiguchi, T.J. Konno, Y. Kawazoe, A. Kumar, U.V. Waghmare	Heating-up and cooling-down molecular-dynamics simulations of 90-degree domain structures in $PbTiO_3$	Domains
PS04	C.M. Schlepütz, Y. Yang, C. Adamo, D.G. Schlom, R. Clarke	Stripe domain evolution in ultrathin $BiFeO_3$ films grown on $TbScO_3$ (110)	Domains
PS05	T. Sluka, A.K. Tagantsev, D. Damjanovic, M. Gureev, N. Setter	Enhanced Electromechanical Response of Ferroelectrics Due to Charged Domain Walls	Domains
PS06	Z. Zhao, J. Blendell, K. Bowman, R. Edwin Garcia	Modeling Domain Dynamics in Single- and Polycrystalline Ferroelectrics	Domains
PS07	R. Adhikari, H. Fu	Electronic structure of LaO doped $SrTiO_3$	Modeling
PS08	S. Amisi, E. Bousquet, K. Katcho, P. Ghosez	First-principles study of structural and vibrational properties of $SrZrO_3$	Modeling
PS09	Y. Cao, S. Bhattacharya, C.A. Randall, L.Q. Chen	Phase-field modeling of resistance degradation and I-V characteristics in perovskite-based ferroelectric oxides	Modeling
PS10	R. Grigalaitis, S. Lapinskas, J. Banys, E.E. Tornau	Dynamics of Relaxation Times in the Three-Dimensional Ising Model	Modeling
PS11	R. Herchig, K. Schultz, K. McCash, I. Ponomareva	Terahertz Frequency Dynamics of Ferrolectric Nanowires	Modeling
PS12	S. Liu, T. Hiroyuki, I. Grinberg, A.M. Rappe	Development of Classical Potential for $PbTiO_3$	Modeling
PS13	N. Ng, K. Bhattacharya	Multiphysics model of semiconducting ferroelectrics and its application to memory devices	Modeling
PS14	A. Prikockytė, C. Dubourdieu, P. Ghosez	Role of electrical and mechanical boundary conditions on the ferroelectric properties of $YMnO_3$ epitaxial thin films	Modeling
PS15	A. Raeliarijaona, H. Fu	Response of zone-center phonon structure to epitaxial strain in $BaTiO_3$	Modeling
PS16	D. Rahmedov, L. Bellaiche, D. Wang, J. Iniguez	Magnetic cycloid of $BiFeO_3$ from atomistic simulations	Modeling
PS17	M. Rose, R.E. Cohen	The Electrocaloric Effect and the Relationship Between Homogenous Polarization Switching and Phase Transitions in Ferroelectrics	Modeling
PS18	S. Subramanian, T. Ozaki, K. Yamauchi, T. Oguchi, N. Baskaran	A first principle structure dynamics study of doping lone pair A cations to $HoMnO_3$	Modeling
PS19	L.F. Wan, T. Nishimatsu, S.P. Beckman	The piezoelectric tensor components of the known phases of $KNbO_3$ calculated by first-principle methods	Modeling
PS20	N. Barrett, J. L. Wang, A. Pancotti, P. Jégou, G. Niu, B. Gautier, Y.Y. Mi, L. Tortech, S. Yin, B. Vilquin	Ferroelectricity in Quasi-Amorphous BaTiO3 Ultra-thin Film	Novel Materials

PS21	J.W. Bennett, K.F. Garrity, K.M. Rabe, D. Vanderbilt	Switchable polarization in stuffed wurtzite compounds, a new class of ferroelectrics	Novel Materials
PS22	V.R. Cooper, S. Takagi, D.J. Singh	First principles prediction of morphotropic phase boundaries in Bi-based ferroelectrics	Novel Materials
PS23	S. Ducharme	Applications of ferroelectric polymer and oligomer thin films	Novel Materials
PS24	C. Fancher, J.E. Blendell, K.J. Bowman	Poling Induced Fatigue in <100> Textured Lead-Free Piezoelectric $Na_{0.5}Bi_{0.5}TiO_3$ (NBT)	Novel Materials
PS25	A.T. Mulder, N.A. Benedek, C.J. Fennie	Crossover between hybrid improper ferroelectricity and proper ferroelectricity in layered perovskites	Novel Materials
PS26	W. Ren, Y. Yang, W. Chen, L. You, Z. Chen, Y. Qi, X. Zou, J. Wang, T. Sritharan, P. Yang, L. Chen, L. Bellaiche	Sm-doped $BiFeO_3$ films under compressive strain	Novel Materials
PS27	S.K. Saha, P. Ghosez	Structural, electronic, and vibrational properties of chloride-based perovskites : A first-principles study	Novel Materials
PS28	Z. Gui, S. Prosandeev, L. Bellaiche	Properties of epitaxial (110) $BaTiO_3$ films from first principles	Phase Transitions
PS29	D. K. Jackson, R. Pattnaik, J. Toulouse	Temperature evolution of the linear birefringence in striated single crystals of $KTa_{1-x}Nb_xO_3$ (KTN)	Phase Transitions
PS30	F. Kadlec, C. Kadlec, P. Kuzel, J. Petzelt	Ferroelectric phase transition in GeTe studied by time-domain THz spectroscopy	Phase Transitions
PS31	A. Kvasov, A. Tagantsev	Can we trust the temperature - misfit strain thin film phase diagrams?	Phase Transitions
PS32	K. McCash, A. Srikanth, I. Ponomareva	Polarization Reversal in Ultrathin Ferroelectric Nanowires under High Electric Fields	Phase Transitions
PS33	Y. Xie, A.A. Bokov, X. Long, Z.-G. Ye	Studies of Domain Structure and Phase Transitions in $PbZr_{1-x}Ti_xO_3$ Single Crystals	Phase Transitions
PS34	M. Ahart, S. Kojima, Z.-G. Ye, R.J. Hemley	Structural transition in $Pb(In_{1/2}Nb_{1/2})O_3$ under pressure	Relaxors
PS35	A. Al-Barakaty, L. Bellaiche	The effects of Oxygen vacancies on properties of PMN-25%PT: a first-principles-based study	Relaxors
PS36	P. Ondrejkovic, M. Kempa, J. Hlinka, J. Kulda, H. Luo, Q. Zhang	Waterfall anomaly in $(Na_{0.5}Bi_{0.5})_{0.96}Ba_{0.04}TiO_3$ single crystal	Relaxors
PS37	H. Takenaka, I. Grinberg, A.M. Rappe	Molecular Dynamics Study of Local Structure and Dynamics in a Relaxor Ferroelectric	Relaxors
PS38	S.J. Callori, J. Gabel, D. Su, J. Sinsheimer, M.V. Fernandez-Serra, M. Dawber	Compositional inversion symmetry breaking in $PbTiO_3/SrRuO_3$ superlattices	Superlattices
PS39	R.S. Katiyar, N. Ortega, A. Kumar	Ferroelectric and Dielectric Properties of $BaTiO_3/Ba_{(1-x)}Sr_xTiO_3$ Superlattices	Superlattices
PS40	J. Sinsheimer, S.J. Callori, Y. Benkara, B. Bein, J. Daley, D. Su, M. Dawber	Engineered polarization rotation in $PbTiO_3/CaTiO_3$ superlattices	Superlattices
PS41	Y. Yang, W. Ren, M. Stengel, X.H. Yan, L. Bellaiche	Phase transitions in epitaxial $PbTiO_3/BiFeO_3$ superlattice from first principles	Superlattices
PS42	V. Železný, C. Kadlec, A. Soukiassian, X.X. Xi, D.G. Schlom	Folded acoustic phonons in infrared spectroscopy of $BaTiO_3/SrTiO_3$ superlattices	Superlattices
PS43	J. Banys, S. Rudys, M. Ivanov, R. Grigalaitis, N.P. Vyshatko, A.D. Shilin, A.N. Salak	Meyer-Neldel rule for electrical conductivity observation in xNBT–(1-x)LMT ceramics	Techniques

PS44	E. Buixaderas, I. Gregora, J. Hlinka, J. Dec	Raman and IR phonons in $Sr_xBa_{1-x}Nb_2O_6$ single crystals	Techniques
PS45	I.S. Golovina, B.D. Shanina, I.N. Geifman	EPR study of $KTaO_3$:Mn nanopowder	Techniques
PS46	N. Inoue, R.A. Maier, A. Honda, H. Takagi, C.A. Randall	Evaluation of defect dipole dissociation energy in rare earth and magnesium co-doped $BaTiO_3$ by TSDC (Thermally Stimulated Depolarization Current) measurement	Techniques
PS47	Y.-M. Kim, M.D. Biegalski, J. He, H.M. Christen, S.T. Pantelides, S.J. Pennycook, A.Y. Borisevich	Direct Atomic-Scale Measurement of Oxygen Stoichiometry in Cobaltite Thin Films	Techniques
PS48	J.H. Lee, S.-H. Chang, I.C. Tung, S.M. Nakhmanson, J. Eastman, D. Fong, H. Hong, J.W. Freeland	Development of molecular-beam epitaxy for in-situ synchrotron x-ray study of layered complex oxides	Techniques
PS49	B. Ma, M. Narayanan, S. Liu, S. Chao, S. Tong, U. Balachandran	Ferroelectric PLZT Films Grown on Metal Foils by Chemical Solution Deposition	Techniques
PS50	I. C. Tung, J. Liu, B. Gray, J. Chakhalian, J.M. Rondinelli, E.A. Karapetrova, J.H. Lee, M.J. Bedzyk, J.W. Freeland	Influence of Symmetry on the Octahedral Rotations of Epitaxial $RNiO_3$ Thin Films	Techniques
PS51	Y. Yang, C.M. Schlepütz, C. Adamo, D.G. Schlom, R. Clarke	Structural Investigation of Ultrathin $BiFeO_3$ Films on $SrTiO_3$ (001) Substrates	Techniques

Withdrawn:

	E. Iolin	Neutron Scattering by the Transverse Optic Wave in Relaxors. Effect of Interaction between TOW Vortex and Polarized Nano Regions	Relaxors