

17:00 19:30 Reception and registration at Carnegie Institution of Washington, 1530 P Street, N.W., Washington, D.C.

Monday, February 4, 2002

Radisson Barcelo Hotel, 2121 P Street, N.W., Washington, DC 20037

8:30 9:00 Registration

9:00 9:10 Introduction: Ronald Cohen

First-principles: Chair, Ronald Cohen

| | | | | |
|-------|-------|---|---|--|
| 9:10 | 9:30 | <u>D.J. Singh</u> , S.V. Halilov and M. Fornari | Naval Research Laboratory and Center For Piezoelectrics By Design Rutgers University | Trends in the Lattice Instabilities Underlying Piezoelectricity |
| 9:30 | 9:50 | <u>J. B. Neaton</u> and K. M. Rabe | Rutgers University | Enhanced Polarization in Strained BaTiO ₃ /SrTiO ₃ Superlattices From First Principles |
| 9:50 | 10:10 | <u>Henry Krakauer</u> and Michael Wu | College Of William and Mary | First-Principles Calculations of Piezoelectricity and Polarization Rotation In PZT |
| 10:10 | 10:35 | Coffee break | | |
| 10:35 | 10:55 | <u>C. Stephen Hellberg</u> | Naval Research Laboratory | First-Principles Calculations of SrTiO ₃ /(Ba,Sr)O/Si with Realistic Interfaces |
| 10:55 | 11:15 | <u>A. Filippetti</u> and N. A. Hill | University Of California Santa Barbara | A Theoretical Study on the Coexistence of Ferroelectricity and Magnetism In Hexagonal Manganites |
| 11:15 | 11:35 | <u>Huaxiang Fu</u> | Department Of Physics/Rutgers University | Pressure Effect and Optical Anisotropy In Piezoelectric Pb(Zr _{0.5} Ti _{0.5})O ₃ |
| 11:35 | 11:55 | <u>Ilya Grinberg</u> , Valentino R. Cooper, and Andrew M. Rappe | University Of Pennsylvania | Local Structure and Phase Transitions in PZT |
| 12:00 | 13:00 | Lunch | | |

Potentials and effective Hamiltonians: Chair, Karin Rabe

| | | | | |
|-------|-------|--|---|---|
| 13:00 | 13:20 | <u>M. Sepliarsky</u> and R.E. Cohen | Carnegie Institution Of Washington | Development of a Shell-Model Potential for Molecular Dynamics for PbTiO ₃ by Fitting First-Principles Results |
| 13:20 | 13:40 | Qingsong Zhang, Mustafa Uludogan, Alejandro Strachan, Tahir Cagin, and <u>William A. Goddard III</u> | <i>Invited</i> California Institute Of Technology | Polarizable Reactive Force Fields for Molecular Dynamics Simulation of Ferroelectrics |
| 13:40 | 14:00 | <u>Jorge Iniguez</u> and David Vanderbilt | Rutgers University | Temperature-Pressure Phase Diagram of BaTiO ₃ |
| 14:00 | 14:20 | <u>Eric Cockayne</u> , Benjamin P. Burton, and Umesh Waghmare | NIST | Effect of Ordered Microdomains on the Properties of PbSc _{1/2} Nb _{1/2} O ₃ : A First Principles Effective Hamiltonian Study |
| 14:20 | 14:40 | <u>L. Bellaiche</u> , Alberto Garcia, A.M. George, Jorge Iniguez and David Vanderbilt | <i>Invited</i> University Of Arkansas | Electric-Field Induced Polarization Paths and Active Optical Phonons In Perovskite Alloys |
| 14:40 | 15:00 | Coffee break | | |

Local structure and dynamics: Chair Peter Davies

| | | | | | |
|-------|-------|---|----------------|--|--|
| 15:00 | 15:20 | <u>Robert Blinc</u> , Bo'Tjan Zalar, Janez Dolin'Ek, Raymond Kind, Paola Maria Cereghetti, and Christian Anton Jeitziner | <i>Invited</i> | J. Stefan Institute | Slater Ice Rules and Takagi Group Motion In Deuteron Glasses |
| 15:20 | 15:40 | <u>V. Hugo Schmidt</u> and Darin J. Arbogast | | Montana State University | Fractal Model for Dielectric Properties of Drap Deuteron Glass |
| 15:40 | 16:00 | <u>P. M. Gehring</u> , S. Wakimoto, K. Hirota, C. Stock, Z.-G. Ye, and G. Shirane. | <i>Invited</i> | National Institute Of Standards and Technology | Ferroelectric Ordering and Soft Modes In $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ |
| 16:00 | 16:20 | <u>S. A. Safrona</u> , E. A. Akhadovb, L. A. Boatner, F. A. Flahertyd, J. A. Lib, T. W. Trelenberg, J. G. Skofronickb and D. H. | | Florida State University | Structural and Dynamic Behavior of $\text{KTa}_{1-x}\text{Nb}_x\text{O}_3$ (001) Surfaces Investigated by Helium Scattering Experiments |
| 16:20 | 16:40 | <u>Carol Thompson</u> , S. K. Streiffer, G. B. Stephenson, J. A. Eastman, D. Fong, O. Auciello, G -R. Bai, M. E. M. Aanerud | | Northern Illinois University | Observation of 180° Stripe Domains in Ferroelectric PbTiO_3 Thin Films |
| 16:40 | 17:00 | <u>D. La-Orautapong</u> , J. Toulouse, Z-G. Ye, R. Erwin, and J.L. Robertson | | Lehigh University | Diffuse Neutron Scattering Study of the Relaxor Ferroelectric $(1-X)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - XPbTiO_3 (PZN-Xpt) |
| 17:00 | 17:20 | Pavol Juhas and <u>Peter K. Davies</u> | | University Of Pennsylvania | Chemical Order and Dielectric Properties in Tungstate Relaxor Perovskites |
| 17:20 | 17:40 | <u>S. B. Vakrushev</u> | <i>Invited</i> | Ioffe Physico-Technical Institute | Structure and Lattice Dynamics of Cubic Relaxor Ferroelectrics |
| 17:40 | 18:00 | <u>Q. M. Zhang</u> , Z. Y. Cheng, Dana Olson | | Penn State University | Relaxor Ferroelectric Polymers |

18:00 19:00 Dinner

Tuesday, February 5, 2002

Local structure and dynamics continues: Chair Takeshi Egami

| | | | | | |
|------|-------|---|----------------|--------------------------------|--|
| 9:00 | 9:20 | <u>Igor A. Kornev</u> and Laurent Bellaiche | | University Of Arkansas | Incommensurate Phases in Perovskites |
| 9:20 | 9:40 | <u>Y. Yacoby</u> | <i>Invited</i> | Hebrew University of Jerusalem | Ferroelectricity in doped incipient ferroelectrics |
| 9:40 | 10:00 | Coffee Break | | | |

Electromechanical and dielectric response: Chair Takeshi Egami

| | | | | | |
|-------|-------|--|----------------|------------------------------------|---|
| 10:00 | 10:20 | <u>Annette Bussmann-Holder</u> , Helmut Büttner and Alan R. Bishop | <i>Invited</i> | Max-Planck-Institute | Precursor Effects, Elastic Anomalies and Acoustic Mode Instabilities in SrTiO_3 |
| 10:20 | 10:40 | Eugene Heifet, <u>Ronald E. Cohen</u> and H. Fu | | Carnegie Institution Of Washington | Ab Initio Study of Elastic Properties of $\text{Pb}(\text{Zr,Ti})\text{O}_3$ |
| 10:40 | 11:00 | <u>Karin A. Rabe</u> | | Rutgers University | Polarization and Dielectric Response of Atomic-Scale Perovskite Heterostructures by Design |
| 11:00 | 11:20 | <u>David Vanderbilt</u> , Lixin He, J.B. Neaton, Morrel H. Cohen | | Rutgers University | Theory Of The Dielectric Response of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ |
| 11:20 | 11:40 | <u>P. Chandra</u> , M. Dawber, P.B. Littlewood, J.F. Scott and M.M.J. Treacy | | NEC Research Institute | Frequency-Dependence of Coercive Fields in Ferroelectric Films |
| 11:40 | 12:00 | M. Sepiarsky; <u>S. R. Phillpot</u> , M. G. Stachiotti and R. L. Migioli | | Argonne National Laboratory, | Dynamics Of Polarization Rotation and Homogeneous Domain Nucleation In A Perovskite Ferroelectric By Molecular-Dynamics Simulations |

12:00 13:00 Lunch

| | | | | |
|-------|-------|--|--|--|
| 13:00 | 13:20 | <u>S. Prosandeev</u> , V. Trepakov, S. Kapphan, M. Savinov, B. Burton, and E. Cockayne | National Institute Of Standards and Technology | Dielectric Response in Microscopically Heterogeneous Dielectrics: Examples of KTN and KTL |
| 13:20 | 13:40 | <u>Jaichan Lee</u> , Juho Kim, Young Sung Kim, Leejun Kim, and Donggeun Jung | Sung Kyun Kwan University | Dielectric Properties of BaTiO ₃ /SrTiO ₃ Oxide Superlattice |
| 13:40 | 14:00 | <u>Rui Zhang</u> , Bei Jiang and Wenwu Cao | Penn State University | Elastic, Dielectric and Piezoelectric Coefficients for Domain Engineered 0.70Pb(Mg _{1/3} Nb _{2/3})O ₃ -0.30PbTiO ₃ Single Crystal |

Polarization and effective charges: Chair: David Vanderbilt

| | | | | |
|-------|-------|--|---------------------------------------|--|
| 14:00 | 14:20 | <u>R. Resta</u> and Alfredo Pasquarello | <i>Invited</i> Universita' di Trieste | A generalization of the effective-charge concept: Dynamical multipoles In molecular solids and liquids |
| 14:20 | 14:40 | <u>Marek Veithen</u> | Universite De Liege | Electron Localization In Ferroelectric Oxides |
| 14:40 | 15:00 | <u>T. Egami</u> , E. Mamontov and W. Dmowski, University Of Pennsylvania, T. Gog and C. Venkataraman, Argonne National | University Of Pennsylvania | Electronic States of Ferroelectric Oxides Probed by X-Ray Spectroscopy and Scattering |

15:00 15:20 Coffee break

Films and ceramics: Chair David Vanderbilt

| | | | | |
|-------|-------|--|-----------------------------------|--|
| 15:20 | 15:40 | <u>Jiangyu Li</u> | University Of Nebraska-Lincoln | A Mesoscopic Electromechanical Theory of Ferroelectric Films and Ceramics |
| 15:40 | 16:00 | <u>Magali Zimmer</u> , Javier Junquera, and Philippe Ghosez | Universite De Liege | Structural and Electronic Properties of Nanosized Ferroelectric Films |
| 16:00 | 16:20 | <u>Stephen Ducharme</u> , G. Visdrik, A. V. Sorokin, V. M. Fridkin | University Of Nebraska | Intrinsic Switching Kinetics In Ferroelectric Copolymer Films |
| 16:20 | 16:40 | <u>X. X. Xi</u> | The Pennsylvania State University | Nature of Phase Transitions in Ba _x Sr _{1-x} TiO ₃ Thin Films |

16:40 18:30 Poster session: Chair Andrew Rappe

18:30 19:30 Dinner

Wednesday, February 6

Surfaces, Defects and domains: Chair. Henry Krakauer

| | | | | |
|------|-------|---|--|---|
| 9:00 | 9:20 | <u>A.M. Bratkovsky</u> and A.P. Levanyuk | Hewlett-Packard Laboratories | Formation and Rapid Evolution of Domain Structure at Phase Transitions in Slightly Inhomogeneous Ferroelectrics |
| 9:20 | 9:40 | <u>Terrence Jach</u> , Sungwon Kim, Venkatraman Gopalan, Stephen Durbin, and David Bright | National Institute Of Standards and Technology | Surface Behavior of Congruent LiNbO ₃ Domains under the Action of Applied Fields |
| 9:40 | 10:00 | <u>Alexander L. Roytburd</u> and Julia Slutsker | University Of Maryland | Elastic Domain Architectures in Constrained Ferroelectric Films |

10:00 10:20 Coffee break

| | | | | |
|-------|-------|--|-------------------------------|---|
| 10:20 | 10:40 | S. Kim, T. Jach, S. Durbin, Venkatraman <u>Gopalan</u> | Pennsylvania State University | The Role of Defects on Local Domain Wall Structure and its Movement in Ferroelectrics |
| 10:40 | 11:00 | <u>Wenwu Cao</u> | Pennsylvania State University | Revisit Polarization Reversal Mechanism Using Ultrasound |

Posters

| | | |
|--|--|---|
| <u>Rajeev Ahluwalia</u> and Wenwu Cao | Los Alamos National Lab | Simulation Study of Surface Effects in Constrained Ferroelectrics |
| <u>Peter K. Davies</u> , Irina Molodetsky, Albina Borisevich | University Of Pennsylvania | New Examples of Cation Order in Perovskite Oxides |
| Ilya Grinberg, <u>Valentino R. Cooper</u> , and Andrew M. Rappe | University Of Pennsylvania | Dft and Monte Carlo Studies of PZT Local Structure |
| <u>W. Dmowski</u> , E. Mamontov, T.Egami, S. Vakrushev | University Of Pennsylvania | X-ray Diffuse Scattering from Doped Single Crystal KTO |
| <u>E. Heifets</u> , R.I. Eglitis, E.A. Kotomin, D. J. Maier, and G. Borstel | Carnegie Institution Of Washington | First-Principles Calculations for SrTiO ₃ (100) Surface Structure |
| <u>Gina L. Hoatson</u> , Donghua H. Zhou, Franck Fayon, Dominique Massiot, Robert Vold and Zhehong Gan | College Of William and Mary | Solid State Multinuclear NMR Studies of Relaxor Ferroelectrics |
| <u>Jorge Iniguez</u> , J. B. Neaton, and David Vanderbilt | Rutgers University | Effective-Hamiltonian Modeling of External Pressure in Ferroelectric Perovskites |
| <u>Matt Poulsen</u> , S. Adenwalla, Stephen Ducharme, V. M. Fridkin, S. P. Palto, N. N. Petukhova, and S. G. Yudin | University Of Nebraska | Use of an External Electric Field to Convert the Paraelectric Phase to the Ferroelectric Phase in Ultrathin Copolymer Films |
| <u>S. A. Prosandeev</u> , E. Cockayne and B. Burton | National Institute Of Standards and Technology | Properties of Prototype Solid Solutions of KNbO ₃ , KTaO ₃ and LiTaO ₃ on the Basis of First-Principle Computations and Experiment |
| I. P. Raevski and <u>S. A. Prosandeev</u> | | A New Lead-Free Family of Perovskites with Diffuse Phase Transitions: NaNbO ₃ - Based Solid Solutions |
| <u>Na Sai</u> , Karin M. Rabe and David Vanderbilt | Rutgers University | Theory of Structural Response to External Electric Field in Ferroelectric Systems |
| <u>S. Savrasov</u> | New Jersey Institute of Technology | Importance of correlation effects in lattice dynamics of NiO |
| <u>S.K. Streiffer</u> , Carol Thompson, G.B. Stephenson, J.A. Eastman, D. Fong, M.V.R. Murty, A. Munkholm , M. E. M. | Argonne National Laboratory | In-Situ Synchrotron X-Ray Studies of Metal-Organic Chemical Vapor Deposited PbTiO ₃ Thin Films |
| <u>Silvia Tinte</u> , J. Iniguez, K. Rabe and D. Vanderbilt | Rutgers University | Testing an effective Hamiltonian for BaTiO ₃ using an atomistic model |
| <u>Yizhak Yacoby</u> | Hebrew University | Direct Determination of The Atomic Structure of Systems With Two-Dimensional Periodicity |