

2016 Workshop on the
Fundamental Physics of Ferroelectrics and Related Materials
31 January – 3 February, 2016

PROGRAM

Carnegie Institution of Washington
1530 P Street NW, Washington, DC
(Please use the entrance on P Street)

Registration:	Ballroom
Reception, Banquet, Buffet Dinner:	Ballroom
Lectures:	Auditorium
Poster Session:	Rotunda
WiFi Access:	Network = Carnegie_Public Password = jupiter123456789

SUNDAY – 31 JANUARY, 2016

**REGISTRATION AND RECEPTION – 17:00 to 19:00
(BALLROOM)**

MONDAY – 1 FEBRUARY, 2016

**OPENING REMARKS – 07:50 to 08:00
(AUDITORIUM)**

MONDAY MORNING – 1 FEBRUARY, 2016
(AUDITORIUM)

Relaxors: 08:00 to 10:00 (Chair – A Bussmann-Holder)

- 08:00 S Vakhrushev – Dielectric freezing in the lead-free relaxor $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$
- 08:20 S Kojima – Relaxor-like behavior of ferroelectric phase transitions in $\text{K}(\text{Ta}_{1-x}\text{Nb})\text{O}_3$ crystals
- 08:40 M Manley – Complex dynamical patterns emerging from 3-phonon coupling in a relaxor ferroelectric
- 09:00 P Gehring – On phonon localization in relaxors
- 09:20 A Bosak – Diffuse scattering in $\text{Sr}_{0.6}\text{Ba}_{0.4}\text{Nb}_2\text{O}_6$: three faces of disorder
- 09:40 I Grinberg – Similarities between the structure, dynamics, and dielectric properties of perovskite oxide relaxor ferroelectrics and water

MORNING COFFEE BREAK – 10:00 to 10:30

Improper Ferroelectrics: 10:30 to 12:00 (Chair – J Rondinelli)

- 10:30 M Senn (INVITED) – From improper ferroelectrics to negative thermal expansion – what symmetry analysis of competing crystallographic phases can tell us about dynamics
- 11:00 S Kamba – High-temperature electromagnons in Z-type hexaferrite $(\text{Ba}_x\text{Sr}_{1-x})_3\text{Co}_2\text{Fe}_{24}\text{O}_{41}$ and ferroelectric soft mode in improper ferroelectric 2H-BaMnO_3
- 11:20 F-T Huang – Domain topology and conducting ferroelectric walls in a hybrid improper ferroelectric
- 11:40 X-Z Lu – First-principles study of the layered oxides with hybrid improper ferroelectricity

LUNCH (on your own) – 12:00 to 13:30

Magnetoelectrics: 13:30 to 14:50 (Chair – P Maksymovych)

- 13:30 N Bristowe (INVITED) – Coupling and electrical control of structural, orbital, and magnetic orders in perovskites
- 14:00 A Grutter (INVITED) – Probing magnetoelectric heterostructures with polarized neutron reflectometry
- 14:30 A Morelli – Deterministic polarization switching in multiferroic bismuth ferrite nanoislands for magnetoelectric memories

AFTERNOON COFFEE BREAK – 14:50 to 15:20

**MONDAY AFTERNOON – 1 FEBRUARY, 2016
(AUDITORIUM)**

Lead-Free Oxide Perovskites: 15:20 to 17:00 (Chair – Z Ye)

- 15:20 V Cooper (INVITED) – Designing high response lead-free piezoelectrics: From first principles
15:50 O Diéguez (INVITED) – First-principles prediction of supertetragonal phases in perovskite oxide films:
the case of BiMnO_3
16:20 H Moriwake – First-principles calculations of electric-field induced ferroelectric phase transition in
 AgNbO_3
16:40 JH Lee – Record-high ferroelectric polarization by spins and non-reciprocal directional dichroism in
 BiFeO_3

SHORT BREAK – 17:00 to 17:20

High-Throughput/Efficient First Principles Calculations: 17:20 to 18:20 (Chair – D Vanderbilt)

- 17:20 K Garrity – High-throughput first-principles search for new ferroelectrics
17:40 J Bonini – Efficient computation of spontaneous polarization using Wannier center displacements
18:00 J Sun – Accurate geometric and energetic properties of ferroelectric and related materials from an
efficient density functional

BANQUET (BALL ROOM) – 19:30 to 21:30

TUESDAY MORNING – 2 FEBRUARY, 2016
(AUDITORIUM)

Domains and Domain Walls: 08:00 to 10:10 (Chair – N Barrett)

- 08:00 S Liu (INVITED) – Understanding the dynamics of ferroelectric domain walls with MD simulations
08:30 J Chapman – Novel ferroelectric nanobubble domains in strained prototypical thin films
08:50 G Nataf – Experimental evidence of defects stabilized by neutral domain walls
09:10 V Garcia – Learning through ferroelectric domain dynamics in solid-state synapses
09:30 A Bokov – Observation of domain wall dynamics in ferroelectrics by means of x-ray photon correlation spectroscopy
09:50 B Wang – Complex nano/micro domain structure in tetragonal $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ single crystals

MORNING COFFEE BREAK – 10:10 to 10:40

Energy Materials and Applications: 10:40 to 12:00 (Chair – E Bousquet)

- 10:40 B Dkhil – Towards improved caloric responses using ferroelectrics
11:00 J Cuzzo – Piezocaloric effect in antiferroelectric PbZrO_3 from atomistic simulations
11:20 B Xu – Antiferroelectric RE-substituted BiFeO_3 : A lead-free system for large energy storage density
11:40 M Kuklja – Structural (in)stability of complex perovskites for solid oxide fuel cells: First-principles calculations

LUNCH (on your own) – 12:00 to 13:30

Photovoltaics and Novel Perovskites: 13:30 to 15:10 (Chair – B Dkhil)

- 13:30 J Spanier (INVITED) – Semiconducting ferroelectric photovoltaics
14:00 C Stock (INVITED) – From soft harmonic phonons to fast relaxational dynamics in $\text{CH}_3\text{NH}_3\text{PbBr}_3$
14:30 L Tan – Ferroelectric domains in the presence of molecular orientational disorder in hybrid perovskites
14:50 R Cohen – Synthesis and characterization of predicted oxynitride perovskite YSiO_2N

AFTERNOON COFFEE BREAK – 15:10 to 15:40

**TUESDAY AFTERNOON – 2 FEBRUARY, 2016
(AUDITORIUM)**

Advances in Theory/Expt: 15:40 to 17:10 (Chair – H Krakauer)

- 15:40 L Bellaiche (INVITED) – Atomistic simulations of complex problems in ferroelectrics
16:10 P Maksymovych (INVITED) – To switch or not to switch: Another probe microscopy perspective
16:40 M Stengel (INVITED) – First-principles theory of flexoelectricity

SHORT BREAK - 17:10 to 17:30

BaTiO₃-Based: 17:30 to 18:20 (Chair – S Kamba)

- 17:30 E Cockayne – Structure of ultrathin film Ba-Ti-O
17:50 N Barrett – Evolution of surface charge and domain structure through the ferroelectric paraelectric phase transition in BaTiO₃ (001) using MEM-LEEM
18:10 A Everhardt – Ferroelectric domain structures in low-strain BaTiO₃
18:30 S Tsukada – Disorder in BaTiO₃ probed by angle-resolved polarized Raman scattering
18:50 A Grünebohm – *Ab initio* phase diagram of BaTiO₃ under epitaxial strain revisited

POSTER SESSION/BUFFET DINNER – 19:30 to 21:30

**POSTER SESSION
(ROTUNDA)**

Posters should not exceed 3 feet wide by 4 feet high (91 cm by 121 cm). Pins will be provided.

**** ALL posters should remain up from Monday morning through Tuesday evening. ****

1. C Ablitt – Understanding negative thermal expansion in improper ferroelectric Ruddlesen-Popper oxides from first principles
2. A Albarakati – Finite-temperature properties of PMN-25PT nanodots from first principles
3. N Barrett – Charged domain walls and polar boundaries in LiNbO₃ and CaTiO₃ studied by mirror electron microscopy
4. S Bin-Omran – Application of the Wang-Landau Monte-Carlo formalism applied to ferroelectric materials
5. E Bousquet – Proper and improper ferroelectricity in the $n=3$ Dion-Jacobson material $AA_2'Ti_2NbO_{10}$
6. JH Chang – Study of mixed crystals $[N(CH_3)_4]_2Zn_{1-x}Co_xCl_4$ ($x=0, 0.5, 0.7, 0.9, \text{ and } 1$) by NMR
7. C Dreyer – Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides
8. A Dziazgys – Two types of domains in $CuInP_2Se_6$ layered crystals
9. A Everhardt – Transitions between $BaTiO_3$ ca_1/ca_2 and a/c phases
10. H Fu – Mode sequence, frequency change of non-soft phonons, and LO-TO splitting in strained tetragonal $BaTiO_3$
11. O Gindele – Evolution of the local structure of $PbZr_{0.5}Ti_{0.5}O_3$ under applied electric fields
12. E Glazkova – Electrocaloric properties of ferroelectric ultrathin films in the presence of a residual depolarizing field
13. H Hamdi – First-principles re-investigation of bulk WO_3
14. C Hendriks – Mott-Hubbard gap in insulating phases of VO_2 : *ab initio* calculations of the infrared and optical spectra
15. R Herchig – Electrocaloric effect in ferroelectric nanowires from atomistic simulations
16. A Honda – Theoretical study for fundamental physics of low dielectric loss perovskite $Ba(Zn_{1/3}Ta_{2/3})O_3$
17. E Iolin – Resonance damping of the THz-frequency transverse acoustic phonon in the relaxor ferroelectric $K(Ta_{1-x}Nb_x)O_3$
18. Z Jiang – Special quasirandom structures for complex perovskite alloys
19. R Kalfarisi – Investigation of local structure and cation ordering in dielectric oxide microwave ceramics using 7Li and ^{93}Nb solid-state NMR spectroscopy
20. K Kalke – Ultra-large-scale hybrid Monte Carlo simulations of ferroelectric and relaxor materials
21. Karandeep – Exploring the properties of [100], [110], and [111]-oriented vanadate superlattices from first principles
22. E Kotomin – First-principles calculations of oxygen vacancies in the bulk and on the surface of complex perovskites for solid oxide fuel cell cathodes

**POSTER SESSION
(ROTUNDA)**

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23. M Krogstad – Single crystal diffuse scattering study of relaxor $(1-x)\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3-x\text{PbTiO}_3$
24. A Lim – NMR study of Ti- or Fe-doped $\text{LiNbO}_3:\text{Mg}$ single crystals
25. P Maksymovych – Chemical phase-separation in ferroelectric layered transition metal thiophosphates
26. R Nakamoto – First-principles calculations of rare-earth iron garnets
27. J Ouyang – Heterophase polydomain nanostructure in epitaxial ferroelectric films
28. C Paillard – Photostriction in BiFeO_3 from first principles
29. S Park – Charge-order-induced ferroelectricity in $\text{LaVO}_3/\text{SrVO}_3$ superlattices
30. K Patel – Universal energetic coupling in complex antiferroelectric and incommensurate perovskites
31. S Prokhorenko – Symmetry vs topology and dipolar fluctuations in proper ferroelectrics
32. Y Qi – Temperature-driven phase transitions in BaTiO_3 : An atomistic scale description
33. R Qui – Ferroelectric instability in nanotubes and spherical nanoshells
34. S Reyes-Lillo – Effect of hydrostatic strain in the photocatalytic properties of BiVO_4 from first principles
35. H Robinson – ONR's research program on acoustic transduction materials and devices
36. D Saldana-Greco – Improper magnetic ferroelectricity of nearly pure electronic nature in cycloidal spiral $\text{CaMn}_7\text{O}_{12}$
37. S KC – Spin-driven polarization in BiMO_3 ($M=3d$ transition metals) multiferroics: From first principles
38. O Sayedaghaee – Controlling phase coexistence in mixed phase BiFeO_3
39. M Senn – Emergence of long-range order in BaTiO_3 from local symmetry-breaking distortions
40. S Skiadopoulou – Ferroelectric-like poling in paraelectric system
41. I Sluchinskaya – Structure of color centers in BaTiO_3 and SrTiO_3 doped with cobalt
42. S Svirskas – Dielectric, IR, and Raman spectroscopic studies of NBT-based solid solutions
43. H Takenaka – First-principles studies of effects of defects on reversible electro-strain coupling in BaTiO_3
44. N Tillack – *Ab initio* modelling of the magnetoelectric response in Cr_2O_3
45. R Vadapoo – Effect of manganese substitution in barium titanate and PIN-PMN-PT
46. R Walter – Electrical control of chiral phases in electrotoroidic nanocomposites
47. C Wang – Polarization in ferroelectrics
48. F Wang – Effects of oxide on the detonation initiation of energetic materials from first principles
49. Y Yang – Large elasto-optic effect in epitaxial PbTiO_3 films
50. H You – Partial glass isosymmetry transition in multiferroic hexagonal ErMnO_3
51. S Yuk – A first-principles study of ferroelectric PbTiO_3 , BaTiO_3 , and KNbO_3 : Exchange and correlation effects
52. F Zheng – Rashba spin-orbit coupling enhanced carrier lifetime in $\text{CH}_3\text{NH}_3\text{PbI}_3$

WEDNESDAY MORNING – 3 FEBRUARY, 2016
(AUDITORIUM)

Multiferroics: 08:00 to 10:10 (Chair – L Bellaiche)

- 08:00 X Wu (INVITED) – Stabilization of a highly polar BiFeO₃-like structure: A new interface design route for enhanced ferroelectricity in artificial perovskite superlattices
- 08:30 A Bussmann-Holder – Transition metal oxides: Promising candidates for multifunctional applications
- 08:50 J Banys – Broadband dielectric studies of cobalt-ferrite-doped lead zirconium titanate multiferroic composites
- 09:10 F Ricci – Unveiling the room temperature magnetoelectricity of troilite FeS
- 09:30 F Thöle – The macroscopic magnetoelectric monopolization in diagonal magnetoelectrics
- 09:50 Z-G Ye – Ferroelectric and magnetic double morphotropic phase boundaries in Dy-modified BiFeO₃-PbTiO₃ multiferroics

MORNING COFFEE BREAK – 10:10 to 10:40

Advances in Ferroelectrics: 10:40 to 12:50 (Chair – R Cohen)

- 10:40 C Eom (INVITED) – Emergence of room-temperature ferroelectricity at reduced dimensions
- 11:10 D Amoroso – *Ab-initio* approach to structural, electronic, and ferroelectric properties of antimony sulpho-iodide
- 11:30 E Nowadnick – Ferroelectric switching pathways in Ca₃Ti₂O₇ from first principles
- 11:50 M Itoh – Shearing-mediated ferroelectricity: Polarization switching caused by the bond recombination of cations
- 12:10 M Ye – Ferroelectricity in corundum derivatives
- 12:30 Y Nahas – Underlying topological features in ferroelectrics

END OF WORKSHOP