

# KYLE P. KELLEY

Knoxville, TN 37932  
kelleykp@ornl.gov ◊ (828)406-4534

## EDUCATION

---

### North Carolina State University

May 2018

*Doctor of Philosophy*

*Department of Materials Science and Engineering*

Dissertation title: "Mid-infrared plasmonics in cadmium oxide thin films"

Advisor: Professor Jon-Paul Maria

### North Carolina State University

December 2017

*Master of Materials Science and Engineering*

### Appalachian State University

May 2014

*Bachelor of Science in Applied Physics*

## RESEARCH EXPERIENCE

---

### Oak Ridge National Laboratory

April 2021 - Present

*Center for Nanophase Materials Science: Functional Atomic Force Microscopy Group*

*Research and Development Associate (40 hr.s/week)*

- Collaborate with visiting scientists to submit successful DOE user proposals to achieve mission critical objectives.
- Develop automated and dynamic piezoresponse force microscopy techniques to explore ferroelectric and ionic phenomena.
- Leverage ultra-high vacuum scanning probe microscopy to identify material properties dependence on interfacial and defect chemistry.

### Oak Ridge National Laboratory

September 2018 - May 2021

*Center for Nanophase Materials Science: Scanning Probe Microscopy Group*

*Postdoctoral Researcher*

- Implemented pulsed laser deposition (PLD) of ferroelectric complex oxides with in-situ chemical, structural and electronic characterization for fundamental studies.

### North Carolina State University

August 2014 - August 2018

*Graduate Student Researcher (Advisor: Prof. Jon-Paul Maria)*

- Synthesized doped oxide semiconductor thin films with tunable plasmonic modes for high performance infrared detectors.
- Identified promising dopants for the high mobility semiconductor cadmium oxide (yttrium, indium, tin) and feasible growth alternatives (reactive RF co-sputtering and reactive impulse DC co-sputtering).
- Predictive modeling and measuring of plasmonic modes available in oxide thin films (transfer matrix modeling method and infrared optical measurements).
- Built, designed, and implemented high vacuum chambers for the growth of high performance electronic thin films.

### Appalachian State University

August 2011 - May 2014

*Undergraduate Student Researcher (Advisor: Prof. Tonya S. Coffey)*

- Correlated nano-scale thermal properties of organic solar cells to efficiency mechanisms with the use of a Nano-TA2 thermal analysis system in conjunction with atomic force microscopy.

## SKILLS

---

- Experienced in advanced scanning probe microscopy techniques including atomic force microscopy, piezoresponse force microscopy, scanning tunneling microscopy, and Kelvin probe microscopy.
- Proficient in multiple computational platforms including Python, Matlab, Mathematica, Lumerical, AutoCAD, Labview, and Igor.
- Thin film synthesis (PLD, sputtering, and molecular beam epitaxy), infrared and visible spectroscopies, X-ray spectroscopies, scanning electron microscopy, device and thin film electrical characterization.

## PUBLICATIONS

---

### Selected Peer-Reviewed and Published Articles

1) K.P. Kelley, A.N. Morozovska, E.A. Eliseev, Y. Liu, S.S. Fields, S.T. Jaszewski, T. Mimura, S. Calderon, E.C. Dickey, J.F. Ihlefeld, S.V. Kalinin, "Ferroelectricity in Hafnia Controlled via Surface Electrochemical State", *Nat. Mater.*, **22**, 1144–1151 (2023).

1) K.P. Kelley, A.N. Morozovska, E.A. Eliseev, V. Sharma, D.E. Yilmaz, A.C.T. van Duin, P. Ganesh, A. Borisevich, S. Jesse, P. Maksymovych, N. Balke, S.V. Kalinin, R.K. Vasudevan, "Oxygen Vacancy Injection as a Pathway to Enhancing Electromechanical Response in Ferroelectrics", *Adv. Mater.*, 2106426 (2022).

2) K.P. Kelley, Y. Ren, A. Dasgupta, P. Kavle, S. Jesse, R.K. Vasudevan, Y. Cao, L.W. Martin, S.V. Kalinin, "Probing Metastable Domain Dynamics via Automated Experimentation in Piezoresponse Force Microscopy", *ACS Nano*, **15**, 9, 15096-15103 (2021).

3) R.K. Vasudevan, K.P. Kelley, H. Funakubo, S. Jesse, S.V. Kalinin, M. Ziatdinov, "Autonomous Experiments in Scanning Probe Microscopy and Spectroscopy: Choosing Where to Explore Polarization Dynamics in Ferroelectrics", *ACS Nano* **15**, 7, 11253-11262 (2021).

4) O. Paull, C. Xu, X. Cheng, Y. Zhang, B. Xu, K.P. Kelley, A. de Marco, R.K. Vasudevan, L. Bellaiche, V. Nagarajan, D. Sando, "Anisotropic epitaxial stabilization of a low-symmetry ferroelectric with enhanced electromechanical response", *Nat. Mater.* (2021)

5) W. Zhang, S. Cheng, C.M Rouleau, K.P. Kelley, J. Keum, E. Stavitski, Y. Zhu, M.F. Chisholm, Z. Gai, G. Eres, "Unusual electrical conductivity driven by localized stoichiometry modification at vertical epitaxial interfaces", *Mater. Horiz.* **7**, 12, 3217-3225 (2020)

6) K.P. Kelley,\* A. Dziaugys,\* J.A. Brehm, L. Tao, A. Puretzky, T Feng, A. O'Hara, S. Neumayer, M. Chyasnovichyus, E.A. Eliseev, J. Banyas, Y Vysochanskii *et al.*, "Piezoelectric domain walls in van der Waals antiferroelectric CuInP<sub>2</sub>Se<sub>6</sub>", *Nat. Commun.* **11**, 3623 (2020).

7) K.P. Kelley, M. Ziatdinov, L. Collins, M.A. Susner, R.K. Vasudevan, N. Balke, S.V. Kalinin, S. Jesse, "Fast scanning probe microscopy via machine learning: non-rectangular scans with compressed sensing and Gaussian process optimization", *Small* **16**, 2002878 (2020).

8) K.P. Kelley, Y. Ren, A.N. Morozovska, E.A. Eliseev, Y. Ehara, H. Funakubo, T. Giamarchi, N. Balke, R.K. Vasudevan, Y. Cao, S. Jesse, S.V. Kalinin, "Dynamic manipulation in piezoresponse force microscopy: creating non-equilibrium phases with large electromechanical response," *ACS Nano* **15**, 10569-10577 (2020).

9) K.P. Kelley, L. Li, Y. Ren, Y. Ehara, H. Funakubo, S. Somnath, S. Jesse, Y. Cao, R. Kannan, R.K. Vasudevan, S.V. Kalinin, "Tensor factorization for elucidating mechanisms of piezoresponse relaxation via dynamic piezoresponse force spectroscopy", *NPJ Comput. Mater.* **6**, 113 (2020)

10) K.P. Kelley, D.E. Yilmaz, L. Collins, Y. Sharma, H.N. Lee, D. Akbarian, A.C.T van Duin, P. Ganesh, R.K. Vasudevan, "Thickness and strain dependence of piezoelectric coefficient in BaTiO<sub>3</sub> thin films", *Phys. Rev. Materials* **4**, 024407 (2020).

## HONORS AND ACHIEVEMENTS

---

### Awards

- R&D 100 Award. "Physics-Informed, Active Learning-Driven Autonomous Microscopy for Science Discovery" (2023).
- Outstanding Scholarly Output Award. UT-Battelle Awards Night. Oak Ridge National Laboratory (2022).
- Electronic Materials and Applications (EMA) 1st Place Presentation Award. The American Ceramic Society (2018).
- North Carolina Space Grant Recipient. National Aeronautics and Space Administration (2014).

### Patents

- 1) M.A. Ziatdinov, K. Roccapiore, Y. Liu, K.P. Kelley, R.K. Vasudevan, S.V. Kalinin, J.D Hinkle (2022) "Science-Driven Automated Experiments" Provisional application ref. no. 4967.0.
- 2) E. Sachet, C. Shelton, J.P. Maria, K.P. Kelley, E.L. Runnerstrom (2018), "High mobility doped metal oxide thin films and reactive physical vapor deposition methods of fabricating the same" US10741649B2.

## TEACHING AND MENTORING

---

### University of Tennessee Ph.D. Committee Member : Oak Ridge National Laboratory

Committee member for Ph.D. student at University of Tennessee.

### Mentoring Postdoctoral Associate: Oak Ridge National Laboratory

Principal investigator and mentor for postdoctoral associates developing dynamic, time-resolved scanning probe microscopy techniques for materials development.

### ORISE Mentor: Oak Ridge National Laboratory and University of Tennessee

Oak Ridge Institute for Science and Education mentor for Ph.D. student at University of Tennessee.

### Long Term User Mentor: Oak Ridge National Laboratory

Mentoring and educating Lehigh University graduate students.

### Graduate Student Instructor: North Carolina State University

Helped develop and teach undergraduate laboratory classes in X-ray diffraction, calorimetry, and electronic properties of metals and semiconductors.

### Local Outreach Mentor and Instructor: Appalachian State University

Established a mobile nanoscience laboratory outreach program in Western NC that put scanning electron microscopy (SEM) directly in the hands of K-12 students and the general public.

### National Academy of Science Mentor: Appalachian State University

Mentored undergraduates in physics and mathematics.

## INSTRUMENTATION AND FACILITIES

---

- Actively developing various modalities of automated experiments for discovery of new phenomena (w/in AFM and SEM-CL), ultimately enabling a new CNMS user capability.
- Developed laser assisted thermal piezoresponse force microscopy (thPFM) as a new technique available to CNMS users, which enables the measurement of local, temperature induced phenomena.
- Development of NanoIR2 system for IR based nano-spectroscopy and photo-induced functional characterization with increased control of light polarization.

- Maintenance and maintain ultra-high vacuum AFM (wobble stick, heater, stage locker, new HD camera etc.) and ambient AFMs (fixed lasers, upgraded RAM, etc.)
- Laboratory Safety Manager (alt) for scanning probe microscopy laboratories.

## RECENT SCIENTIFIC ACTIVITY

---

### Funding (2023)

- Lead PI on Energy Frontier Research Center (EFRC) program - 3D Ferroelectric Memory (3DFeM) - funded by the DOE
- EFRC Executive committee member tasked with managing center
- ORII Seed Proposal: “High Throughput Synthesis of 2D-Heterostructured Perovskites for Advanced Infrared Sensing and X-ray Imaging Applications” (Co-PI, Submitted)
- ACCELERATE INNOVATIONS IN EMERGING TECHNOLOGIES Proposal: “Controlling Solid-State Emitters for Scalable Quantum Networks” (Co-PI, Submitted)

### Conference/Symposium Organization (2022-2023)

- Co-organized the AI-ML workshop at CNMS (greater than 250 attendees)
- Chaired sessions at International Materials Research Congress (IMRC) conference
- Co-organizer for new program manager seminar series titled “Manager Monday” - PSD based informational meetings series - together with Cynthia Jenks.

## RECENT CONFERENCES

---

- 1) Invited talk: “Ferroelectric Response Controlled via Environmental Piezoresponse Force Microscopy”, 2023 International Symposium on Application of Ferroelectrics Meeting
- 2) Invited talk: “Dynamic ferroelectric domain manipulation via automated experimentation in piezoresponse force microscopy”, American Physical Society March Meeting 2022
- 3) Invited talk: “Oxygen vacancy injection as a pathway to enhancing electromechanical response in ferroelectrics”, 2022 US-Japan Seminar on Dielectric and Piezoelectric Ceramics
- 4) Contributed talk: “Dynamic ferroelectric domain manipulation via automated experimentation in piezoresponse force microscopy”, Materials Research Society Fall 2021
- 5) Contributed talk: “Oxygen vacancy injection as a pathway to enhancing electromechanical response in ferroelectrics”, Electronic Materials and Applications Conference 2022
- 6) Contributed talk: “Thickness Dependence of Piezoelectric Coefficient in Ultra-thin Epitaxial BaTiO<sub>3</sub> Thin Films”, Electronic Materials and Applications Conference 2021, Orlando FL, January 22nd-24th 2020.