# CNMS Operations: Quarterly Report

**NSRC Name, DOE Laboratory(s)**: Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory (ORNL)
**NSRC Director**: Karren More
**Date**: April 5, 2023
**Period covered:** FY23 Quarter 2: January 1 – March 31, 2023

**1. User Program:**

- 2023 CNMS User Meeting: CNMS User Executive Committee (UEC) scheduled the 2023 CNMS User Meeting for August 7-11, 2023. The 2-day user meeting will be held in downtown Knoxville, TN. Workshops on CryoTEM, Charged Polymers, Autonomous Characterization and Synthesis, and Novel Materials for Neuromorphic Computing will be held in conjunction with the user meeting at the CNMS; lab tours will also be conducted that week.
- Spring 2023B Proposal Call: The Spring proposal call is now open and will close on May 3, 2023.
- Proposal Extensions: The user office initiated the process to review extension requests for the 2022A proposal call - 154 projects were initially approved and 66 applied for and were granted extensions. The new expiration date for extensions is January 31, 2024.
- Active User Proposals as of March 31, 2023: 523 (includes 43 rapid access proposals)
    - Industry-led: 21
    - University-led: 341
    - ORNL Staff-led: 114
    - Other Government Laboratory-led: 11
    - HBCU-led: 3
    - Unique Institutions: 195
    - Average Requested Proposal Time: 40 days
    - Science Categories: Proposal distribution - 45% Materials Science; 16% Engineering; 9% Chemistry; 4% Instrumentation; 6% Polymers; 12% Biological/Life Sciences; 3% Physics; 3% Optics; 1% Earth/Environmental Sciences; 1% Medical

**2. PIs and Technical Staff Supported by FWP:**

- **Numbers:**
    - Number (Headcount) of Staff in CNMS Division (not including post-docs): 72
        - Director: 1 (1.0 FTE)
        - Division Administrative: 1 (1.0 FTE)
        - R&D Staff: 55 (37.1 FTEs)
        - Tech Professionals: 5 (3.0 FTEs)
        - Technicians: 5 (2.6 FTEs)
        - User Office: 2 (1.8 FTEs)
        - Administrative: 5 (supported at the directorate level – not included in headcount)
        - Operations (ES&H): 2 (supported at lab level – not included in headcount)
        - Finance: 1 (supported at lab level – not included in headcount)
    - Total # FTEs supported on CNMS FWP (not including post-docs): 45.8
    - Other funding sources/programs: 9 LDRD projects, 2 BES-MSED-FWPs, 1 BES-SUFD-ECA, 1 BES-SUFD-QIS Infrastructure FWP, 3 BES-SUFD-AI/ML FWPs, QSC, 3 EFRCs, multiple EERE offices (BETO, HFTO, VTO)

- **New Staff Hires:**
  - Jewook Park – R&D Staff, Scanning Tunneling Microscopy (STM) Group; from the Institute for Basic Science, South Korea
  - Ganesh Narasimha – Postdoctoral Research Associate in Data NanoAnalytics (DNA) Group (supported 100% by CNMS FWP)
  - Lynda Amichi – Postdoctoral Research Associate in Materials MicroÅnalysis (MMA) Group (supported 100% by Hydrogen & Fuel Cell Technologies Office) from the Office for Science and Technology, Embassy of France in the USA.
  - Hwangsun (Sunny) Kim – Postdoctoral Research Associate in Scanning Transmission Electron Microscopy (STEM) Group (supported 100% by STEM FWP) from Seoul National University, South Korea
- **Staff Departures:**
  - Zachary Gosser – Technician in Functional Hybrid Nanomaterials (FHN) Group is now the Assistant Operations Staff at CNMS (assumed position vacated by Kevin Harman, who is now CNMS Operations Manager)
  - Jacob Teeter – Postdoctoral Research Associate in STM Group; departed for a research position at the Johannes Kepler University, Linz, Austria
  - Kartik Venkatraman – Postdoctoral Research Associate in STEM Group; departed for a position at Honeywell
- **Honors and Awards:**
  - Andy Lupini – elected Class of 2023 Fellow of the Microscopy Society of America (MSA) for "foundational contributions of theory and practice of aberration-corrected STEM and applications for high-resolution EELS and e-beam fabrication."
  - Yongtao Liu - awarded the 2023 Microscopy Society of America (MSA) Postdoctoral Scholar Award for paper titled "Machine Learning-Driven Autonomous Microscopy for Materials and Physics Discovery."
  - Eva Zarkadoula – received a Service Award by the ORNL Women's Alliance Council, March 2023.
  - Karren More – recognized as one of nine pioneering women in fuel cell research" in the article "The 2022 Applied Physics by Pioneering Women: A Roadmap" in *Journal of Physics D: Applied Physics* **56**, 073001 (2023).
  - Sabine Neumayer – awarded one of ORNL's Early Career Scientist LDRDs representing the Physical Sciences Directorate; this LDRD Pilot Program was initiated in January 2023 and recipients will participate (along with Early Career Award recipients and Distinguished Staff Fellows) in ORNL's Pilot Early Career Program.
  - CNMS Division Awards FY22:
    - CNMS Distinguished Scientific Paper – M. Zachman, V. Fung, F. Polo-Garzon, S. Cao, J. Moon, Z. Huang, D. Jiang, Z. Wu, and M. Chi, "Measuring and Directing Charge Transfer in Heterogeneous Catalysts," *Nature Communications* **13**, 2353 (2022).
    - Best CNMS Patent – Ilia Ivanov, "Low-cost Scalable QCM Array for Environmental Sensing"
    - Outstanding Scientific Contribution – Wonhee Ko, Sang Yong Song, Eugene Dumistrescu, and Peter Maksymovych, "Decay-rate Spectroscopy – New Quantum Probe for QIS and Beyond"

  - Most Notable CNMS User Project – Liangbo Liang and An-Ping Li for "STM and 4-probe STM Investigation of Transition Metal Substitutions in Monolayer $MoS_2$ for Atomic-scale Memory and Spintronic Applications," CNMS2020-B-00362 with University of Texas – Austin
  - CNMS Postdoctoral Award – Yongtao Liu
  - CNMS Technician Support Award – James Burns
  - CNMS Special Team Accomplishment – Kevin Harman, Shawn Reeves, Alexis Williams, Ray Unocic, and Michael Zachman for establishing the Cryo-EM laboratories at ORNL/CNMS

- **Significant Invited Talks:**
  - Rigoberto Advincula, "3D Printing High-performance Composites and Polymers: Sustainable Nanomaterials, $CO_2$ Membranes, and Oil-water Separations," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
  - Miaofang Chi, "Elucidating Charge Transfer and Surface Reconstructions in Heterogenous Catalysts using in situ and 4D-STEM," Gordon Research Conference, Tuscany, Italy, February 12-17, 2023.
  - Miaofang Chi, "Emerging Scanning Transmission Electron Microscopy for Energy Materials," Mountain States Society of Electron Microscopists, Winter Conference, tour speaker for Microscopy Society of America (MSA), Golden, CO, February 23, 2023.
  - Miaofang Chi, "Electron Microscopy Research Enabled by Shape-controlled Nanoparticles," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
  - Miaofang Chi, "Elucidating Interfaces in Energy Materials Using Advanced Scanning Transmission Electron Microscopy (STEM)," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
  - Patrick Collier, "Short-term, Long-term, and Heterosynaptic Plasticity of Memristive and Memcapacitive Lipid Bilayer Membranes for Neuromorphic Applications," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
  - Patrick Collier, "Evidence for Long-term Potentiation in Phospholipid Membranes," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
  - Neus Domingo, "Physical Chemistry of Ferroelectric Oxide Surfaces," 15th International Meeting on Ferroelectrics, Tel Aviv, Israel, March 26-30, 2023.
  - Panchepakesan Ganesh, "Harnessing Electron Correlations and Anharmonicity for Energy Efficient Computing," Electronic Materials and Applications (EMA) 2023 Conference, Orlando, FL, January 17-20, 2023.
  - Panchapakesan Ganesh, "Explaining Stabilization and Switching of Polarization in 2D Cu-thio/seleno-phosphate Ferroelectrics," American Physical Society (APS) March Meeting, Las Vegas, NV, March 5-10, 2023.
  - Panchapakesan Ganesh, "Understanding Phase Transitions in Correlated Quantum Materials," 2nd Quantum Matters in Material Science Workshop at NIST, January 31-February 1, 2023 (Virtual).
  - Jordan Hachtel, "Monochromania: A Look into the New Types of Science Enabled by Ultrahigh Energy Resolution Electron Microscopy," Hassel and Marianne Ledbetter MatSE Colloquium at the University of Illinois - Urbana/Champaign, IL, February 13, 2023.
  - Jordan Hachtel, "Monochromania: A Look into the New Types of Science Enabled by Ultrahigh Energy Resolution Electron Microscopy," Vanderbilt University, Nashville, TN, March 23, 2023.

- Sumner Harris, "Real-time Optical Diagnostics for in situ Feedback during Growth and Transformation of Transition Metal Dichalcogenides with Pulsed Laser Deposition," Electronic Materials and Applications (EMA) 2023 Conference, Orlando, FL, January 17-20, 2023.
- Sumner Harris, "Combining Gas-phase, Structural, and Optical Diagnostics for In situ Feedback and Control During Pulsed Laser Deposition," SPIE Photonics West LASE, San Fransisco, CA, January 28 – February 2, 2023.
- Jingsong Huang, "Theoretical Modeling and Computations of New Materials for Electrochemical Energy Conversion/Storage Devices," Global Energy Meet 2023, Virtual, March 6-10, 2023
- An-Ping Li, "Probing Topologically Protected Quantum States with Scanning Tunneling Microscopy," 48th Conference on the Physics and Chemistry of Surfaces and Interfaces (PCSI-48) at the American Vacuum Society (AVS) Quantum Science Workshop, Redondo Beach, CA, January 15–20, 2023.
- Yongtao Liu, "Machine Learning Driven Automated Scanning Probe Microscopy for Material Discovery: Applications in Ferroelectric and Optoelectronic Materials," American Physical Society (APS) March Meeting, Las Vegas, Nevada, March 5-10, 2023.
- Peter Maksymovych, "Tunneling Andreev Reflection for Quantitative Microscopy of Superconductors with Atomic Resolution," Electronic Materials and Applications (EMA) 2023 Conference, Orlando, FL, January 17-20, 2023.
- Peter Maksymovych, "Tunneling Andreev Reflection for Quantitative Microscopy of Superconductors with Atomic Resolution," Condensed Matter Physics Seminar at University of Tennessee, Knoxville, February 2023.
- Karren More, "The Center for Nanophase Materials Sciences," Presentation at Manager Mondays, Oak Ridge National Laboratory, Oak Ridge, TN, January 30, 2023.
- Jonathan Poplawsky, "Atom-by-Atom Structural Materials Analysis for Alloy Development," Microscopy Society of America Student Council Webinar, February 8, 2023. (Virtual)
- Jonathan Poplawsky, "Uncovering Unique Multi-Principal Element Alloy Properties Using Atom Probe Tomography," 2023 TMS Annual Meeting, San Diego, CA, March 19-23, 2023.
- Q.Q. Ren, "Effect of N and/or B Additions on the Precipitation Kinetics in Isothermally Aged and Creep Ruptured 347H Stainless Steels," 2023 TMS Annual Meeting, San Diego, CA, March 19-23, 2023
- Kinga Unocic, "STEM/SEM Study on the Microstructural Evolution and Deformation Mechanisms of Fe-25Cr-20Ni-1.4Nb-0.2C Steel Fabricated by Laser Powder-bed Fusion," 2023 TMS Annual Meeting, San Diego, CA, March 19-23, 2023.
- Rama Vasudevan, "Reinforcement Learning for Materials Synthesis, Optimization, and Design," Electronic Materials and Applications (EMA) 2023 Conference, Orlando, FL, January 17-20, 2023.
- Rama Vasudevan, "Machine Learning and Automated and Autonomous Microscopy for Uncovering Structure-Property Relationships in Ferroic Oxides," Electronic Materials and Applications (EMA) 2023 Conference, Orlando, FL, January 17-20, 2023.
- Yangyang Wang, "Spatial Correlations of Polymer Dynamics: Going beyond the Paradigm of Time Correlation Analysis," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.

- Zili Wu, "Catalytic Insights into Hydrogen Production and Utilization via New Materials and Tools," Chemistry Department Seminar, University of New Hampshire, March 21, 2023.
- Zili Wu, "Oxidative Dehydrogenation of Propane over supported $VO_x$ Catalysts with $O_2$ or $CO_2$," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
- Michael Zachman, "Challenges and Opportunities for Studying Ionomer-Catalyst Interactions Using Advanced Electron Microscopy," Platinum Group Metal and Platinum Group Metal-free Electrocatalysts: Catalyst/Ionomer Interactions Workshop, Telluride, CO, March 8, 2023
- Eva Zarkadoula, "Effects of Precipitate Size and Spacing on Deformation-induced fcc to bcc Phase Transformation," 2023 TMS Annual Meeting, San Diego, CA, March 19-23, 2023.

**3. Postdocs Supported by FWP**

- Total number of post-docs in CNMS Division: 23 FTEs (in addition, 3 positions have been filled and post-docs are on-boarding; 8 positions are open)
- Number of post-docs supported by CNMS FWP: 5 FTEs (in addition, 1 position has been filled and post-doc is on-boarding, 4 positions are currently open)

**4. Progress and Budget Summary on BES NSRC-supported QIS FWP:**

FWP ERKCZ62 "Precision Atomic Assembly for Quantum Information Science," PI - Art Baddorf

- **Progress:** Following the structure outlined in our proposal, progress continues along three directions: infrastructure and experiment, artificial intelligence/machine learning (AI/ML), and computation and theory. Our new Infinity low-temperature STM has been delivered and is undergoing performance testing. Several visits by the vendor have identified a helium leak that is currently being repaired by the manufacturer. Components for sample cleaning and gas deposition have been installed and metal deposition sources ordered. A staff member was hired for atomic assembly and is waiting on visa approval. Research and vendor discussions are ongoing to develop a complementary cryogenic sample system for STEM. Applications in reinforcement learning for synthesis are ongoing along with interviews for a postdoc dedicated to ML for STM. Theorists have developed a full ab initio treatment of spin-orbit coupling for defects in topological films and implemented new functionality in Quantum Monte Carlo for application to FeSn and similar quantum materials.
- **Publications:** None this quarter
- **Invited Presentations:** one invited presentation by Rama Vasudevan at Electronic Materials and Applications (EMA) Meeting, Orlando FL, January 13-17, 2023.
- **Budget summary:**
  - FTE funded staff/post-docs = 1.09 FTE (no post-docs originally on this project but new position posted in Q1 FY23)
  - (a) Second year of Award - Received $2,000,000 in OPE and $0 in EQU
  - (b) Funds received to date (OPE and EQU) – $5,350,000
  - (c) Funds spent to date (OPE and EQU) - $1,500,392
  - (d) Committed equipment funds - $283,872

**5. Progress and Budget Summary on BES NSRC-supported ECRP FWP:**

FWP ERKCZ55 "Probing Electrons in Electrides and Beyond," PI - Miaofang Chi

- **Progress:** Research on transition-metal trihalides using Cryo-STEM techniques is ongoing. These trihalides, including $CrCl_3$, $RuCl_3$, and $CrI_3$, exhibit interesting quantum behavior at low temperatures. Previous studies based on X-ray and neutron scattering have shown that they undergo a crystal structure transition from monoclinic (C2/m) to rhombohedral ($R\bar{3}$) at around 100-150 K. However, our recent work has revealed that this behavior is only observed in bulk materials, while thin flakes exhibit a more dynamic and layer-number-dependent structural transition. We are now completing a systematic study to investigate the phase transition behavior of each material system as a function of temperature and layer numbers. In the past quarter, we expanded our study to include $RhCl_3$ to investigate if the layer-number dependency is universal to all transition-metal trihalides. $RhCl_3$ is a material that does not exhibit a phase transition in its bulk form. Our initial results show that $RhCl_3$ exhibits different phases in thin flake samples, even at room temperature, which is in contrast to previous reports. We are currently collaborating with ORNL's Valentino Cooper to conduct theoretical calculations that will help us understand the unexpected phase transitions observed in the transition-metal trihalides. A manuscript is being prepared for this work. In the future, we plan to develop an algorithm that can automate the determination of stacking changes in 2D materials from HAADF-STEM image contrast, which will accelerate our understanding of these materials. Additionally, we have initiated a new investigation of the charge transfer behavior at the interfaces of heterogeneous structures involving trihalides. Our initial material is $RuCl_3$/graphene, which is predicted to exhibit superconducting behavior at low temperatures due to interfacial charge transfer. We are currently in the process of preparing specimens for this project.
- **Publications:** none
- **Invited Presentations:** none
- **Budget Summary:**
  - FTE funded staff/post-docs = 1.11/3.03 (since awarded in FY19)
  - First year of Award - FY19 – no new funds received in FY23 Q2
  - Funds received to date (OPE and EQU) – $ 2,099,910.33 (no funds received in FY23)
  - Funds spent to date (OPE and EQU) - $1,057,537.17

**6. Progress on BES SUF-supported Data FWP(s)**

CNMS staff are collaborators on three externally led BES-SUFD Data Projects:

- FWP ERKCZ59 "4D Camera Distillery: From Massive Electron Microscopy Scattering Data" led by LBNL. The overarching project is targeted at artificial intelligence and machine learning (AI/ML) based analysis of the huge datasets that are generated by a new generation of ultra-high speed electron detectors. The new post-doc, Elizaveta Tiukalova, has been assembling EELS data from elements in different valence states and coordinating with the collaborators at LBNL. Acquisition of off-axial EELS signals is continuing.
  - Budget Summary:
    - FTE funded staff/post-docs - 0.32/0.44 FTE
    - First year of Award – FY20 – no new funds received in FY23 Q2
    - Funds received to date (OPE and EQU) – $391,000 OPE; $0 EQU
    - Funds spent to date (OPE and EQU) - $211,509
- FWP ERKCZ60 "A Collaborative Machine Learning Platform for Scientific Discovery" led by LBNL. We have completed the development of the Bayesian optimized spectral recommender system (BOSRS). This approach augments a standard automated experiment setup by enabling a user to vote on individually captured spectra (e.g., "like" or "dislike" or rate 1 to 5), allowing for

the adjustment of a search/optimization trajectory in an automated experiment. This approach has been demonstrated for scanning probe microscopy measurements of $PbTiO_3$ (PTO) thin films. We have also designed a new type of variational autoencoder (VAE) that augments the existing VAE training loss with physical constraints or knowledge of a material system. This approach guides the model training toward a more meaningful feature learning from microscopy data that aligns with physical principles. The resulting phy-VAE model offers an unsupervised method for the effective identification of order parameters amidst other sources of variability. This method has been applied to various materials, including NiO-LSMO, $BiFeO_3$, and graphene, demonstrating its effectiveness in extracting meaningful information from large volumes of imaging data.

- Budget Summary:
  - FTE funded staff/post-docs - 0.34/0.58 FTE
  - First year of Award – FY20 – no new funds received in FY23 Q2
  - Funds received to date (OPE and EQU) – $495,000 OPE; $0 EQU
  - Funds spent to date (OPE and EQU) - $313,110

- FWP ERKCZ61 "A Digital Twin for Spatiotemporally Resolved Experiments" led by ANL. We are developing a ML algorithm that can generate the structure factor for scattering based on the real potential parameters vs. using latent space representations. This makes its interpretation far simpler and more physically intuitive. We also explored space-time evolutions of stress relaxation and angular fluctuations in soft matter liquids using molecular dynamics-based digital twins. The results revealed an interplay between stress-strain and topological degrees of freedom that have not been previously investigated. All correlation functions examined show a two-stage relaxation, with the slower-decaying component being responsible for the fragile temperature variations of the shear viscosity.
  - Budget Summary:
    - FTE funded staff/post-docs - 0.22/0.40 FTE
    - First year of Award – FY20 – no new funds received in FY23 Q2
    - Funds received to date (OPE and EQU) – $270,000 OPE; $0 EQU
    - Funds spent to date (OPE and EQU) - $167,739

**7. Operations Equipment (OPE or EQU) Investments:**

| Instrument or Capability | Description | Cost ($K) | Expected Delivery |
|---|---|---|---|
| SQUID Magnetometer | Replacement | $650 K | Installed; users are accessing |
| Gatan ELSA double-tilt cryo-holder for Nion MAC-STEM | Side entry cryo-holder for new cryo-stage on MAC-STEM | $75 K | Delivered and being used on MAC-STEM |
| Unisoku vector-field mK STM | Ordered as part of original QIS infrastructure project (PI Chris Rouleau) | $1,800 K | Installed; performance assessment underway; user access expected mid-summer FY23 |
| Nion IRIS electron energy loss spectrometer | Ultra-high energy resolution EELS for Nion UltraSTEM 100 | $620 K | Delivery expected summer FY23 - will be retrofit with Dectris direct electron detector |
| Heating/cleaning unit for side-entry holders for JEOL NeoARM STEM | Low-T heating unit to bake/clean holders and samples before insertion in STEM | $60 K | Delivery expected summer FY23 |

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|---|---|---|---|
| JEOL Octa Segmented Annular All-field detector | 9-sector segmented detector for JEOL NeoARM STEM | $230 K | Delivery expected summer FY23 |
| Thermo Fisher Helios Ga+ focused ion beam (FIB) instrument | Support specimen preparation for atom probe and TEM/STEM | $1,200 K | Delivery expected September 2023 |
| Four nodes for CNMS cloud infrastructure | Additional nodes to complete CNMS cloud infrastructure | $125 K | Delivery expected September 2023 |
| AFM to Nanoscope 6 | Replacement AFM for rapidly evaluating 2D samples and thin films | $100 K | Delivery expected September 2023 |

**8. Covid Impact:**

- All ORNL staff returned to working full-time, on-site on May 16, 2022; current community status is LOW.
- CNMS staff continue to work remotely with CNMS users when appropriate.

**9. Safety Updates**:

- None to report

**10. Concerns and Challenges**

- No new challenges to report

**11. Other News**:

- Addis Fuhr – Staff Profile was featured as a DOE Office of Science "Science Headline" on February 17, 2023 https://www.energy.gov/science/listings/science-headlines?page=8
- Patrick Collier - Co-organizer, focus session "Biomaterials and Biointerfaces," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
- Patrick Collier - Co-organizer, focus session "Controlled Assembly of Charged Soft Matter," American Chemical Society (ACS) Spring Meeting, Indianapolis, IN, March 26-30, 2023.
- Neus Domingo - Chair, Publication Committee, 15th International Meeting on Ferroelectricity, Tel Aviv, Israel, March 26-30, 2023.
- Zheng Gai – appointed as Editor-in-Chief of Spin Crossover and SpintronicsSection for *Magnetochemistry*.
- Jordan Hachtel - Organized and hosted the 1st "Impromptu EELS Data Analysis Workshop" at CNMS, Oak Ridge, TN, January 31 – February 2, 2023 for CNMS staff, post-docs, and students.
- Jordan Hachtel – elected as a Director of the Executive Council of the Microanalysis Society (MAS) for 3-year term, 2023-2025.
- Jingsong Huang – appointed Associate Editor for journal *Frontiers in Soft Matter*.
- Andy Lupini – Chair-elect for Microscopy Society of America Focused Interest Group "Aberration-corrected Scanning Transmission Electron Microscopy."
- Karren More – External Advisory Board, Materials Science & Engineering Department, North Carolina State University, January 23, 2023.
- Kinga A. Unocic - Symposium Organizer, "Environmental Degradation of Additively Manufactured Alloys," 2023 Minerals, Metals & Materials Society (TMS) Annual Meeting, San Diego, CA, March 19-23, 2023
- Kinga A. Unocic - Symposium Co-organizer, "Phase Stability in Extreme Environments," TMS Annual Meeting, San Diego, CA, March 19-23, 2023.

- Kinga Unocic - Committee Chair, "Corrosion and Environmental Effects Committee," TMS Annual Meeting, San Diego, CA, March 19-23, 2023.
- Yangyang Wang - Co-organizer "Winter School of SANS Data Analysis" held at the Spallation Neutron Source, Oak Ridge National Laboratory, January 9-13, 2023.
- Yangyang Wang - Co-organizer, invited session "Out-of-equilibrium: Structure and Dynamics of Polymers," American Physical Society (APS) March Meeting, Las Vegas, NV, March 5-10, 2023.
- Yangyang Wang - Co-organizer, focus session "Nonequilibrium Structures and Dynamics of Polymeric Materials," American Physical Society (APS) March Meeting, Las Vegas, NV, March 5-10, 2023.
- Michael Zachman – Co-Chair of new Microscopy Society of America (MSA) Focused Interest Group "Low Temperature Electron Microscopy."
- Eva Zarkadoula – Symposium Co-organizer, "Computational Thermodynamics and Kinetics," TMS Annual Meeting, San Diego, CA, March 19-23, 2023.
- Eva Zarkadoula - Co-organizer, Diversity Breakfast, TMS Annual Meeting, San Diego, March 19-23, 2023.
- Eva Zarkadoula - Interview in VIMAgazino of the Greek Newspaper To Vima about her work on materials and DEI in STEM https://www.tovima.gr/print/vimagazino/eya-zarkadoula/
- Eva Zarkadoula – appointed to the Early Career Editorial Board of journal *Nuclear Materials and Energy*.

**12. Science Supported by FWP**

Three highlights will be submitted in FY23 Q2:

1. E.R. Hoglund,* D.-L. Bao, A. O'Hara, T.W. Pfeifer, M.S.B. Hoque, S. Makarem, J.M. Howe, S.T. Pantelides, P.E. Hopkins,* and J.A. Hachtel,* "Direct Visualization of Localized Vibrations at Complex Grain Boundaries," *Advanced Materials* **35**, 2208920 (2023). DOI: 10.1002/adma.202208920

   CNMS-user co-led collaborative publication: Grain boundaries (GBs) are a prolific microstructural feature that dominates the functionality of a wide class of materials. The functionality at a GB results from the unique atomic arrangements, different from those in the grain, that have driven extensive experimental and theoretical studies correlating atomic-scale GB structures to macroscopic electronic, infrared optical, and thermal properties. In this work, a $SrTiO_3$ GB is examined using atomic-resolution aberration-corrected scanning transmission electron microscopy and ultrahigh-energy-resolution monochromated electron energy-loss spectroscopy, in conjunction with density functional theory. This combination enables the correlation of the GB structure, nonstoichiometry, and chemical bonding with a redistribution of vibrational states within the GB dislocation cores. The new experimental access to localized GB vibrations provides a direct route to quantifying the impact of individual boundaries on macroscopic properties.

2. S.M. Neumayer,* N. Bauer, S. Basun, B.S. Conner, M.A. Susner, M.O. Lavrentovich, and P. Maksymovych,* "Dynamic Stabilization of Metastable States in Triple-Well Ferroelectric $Sn_2P_2S_6$," *Advanced Materials* 2211194 (2023, in press). DOI: 10.1002/adma.202211194

   CNMS-user co-led collaborative publication: Polarization dynamics in ferroelectric materials is governed by the effective potential energy landscape of the order parameter. The unique aspect of ferroelectrics compared to many other transitions is the possibility of more than two potential wells, leading to complicated energy landscapes with new fundamental and functional properties. Here, direct dynamic evidence is revealed of a triple-well potential in the metal thiophosphate $Sn_2P_2S_6$ compound using multivariate scanning probe microscopy combined with theoretical simulations. The key finding is that the metastable zero polarization state can be accessed through a gradual switching process and is stabilized over a broad range of electric fields. Simulations confirm that the observed zero polarization state originates from a kinetic stabilization of the nonpolar state of the triple-well, as opposed to domain walls. Dynamically, the triple-well of $Sn_2P_2S_6$ becomes equivalent to antiferroelectric hysteresis loops. Therefore, this material combines the robust and well-defined

domain structure of a proper ferroelectric with dynamic hysteresis loops present in antiferroelectrics. Moreover, the triple-well enhances mem-capacitive effects in Sn2P2S6, which are forbidden for ideal double-well ferroelectrics. These findings provide a path to tunable electronic elements for beyond binary high-density computing devices and neuromorphic circuits based on dynamic properties of the triple-well.

3. D. Eby, M. Jakowski, V. Lauter, M. Doucet, P. Ganesh,* M. Fuentes-Cabrera,* and R. Kumar,* "Extraction of Interaction Parameters from Specular Neutron Reflectivity in Thin Films of Diblock Copolymers: An Inverse Problem," *Nanoscale* (2023, in press). DOI: 10.1039/d2nr07173h

   CNMS-led publication: Diblock copolymers have been shown to undergo microphase separation due to an interplay of repulsive interactions between dissimilar monomers, which leads to the stretching of chains and entropic loss due to the stretching. In thin films, additional effects due to confinement and monomer–surface interactions make microphase separation much more complicated than in that in bulks (i.e., without substrates). Previously, physics-based models have been used to interpret and extract various interaction parameters from the specular neutron reflectivities of annealed thin films containing diblock copolymers; however, extracting Flory– Huggins $\chi$ parameters characterizing monomer–monomer, monomer–substrate, and monomer–air interactions has been labor-intensive and prone to errors, requiring the use of alternative methods for practical purposes. In this work, we have developed such an alternative method by employing a multilayer perceptron, an autoencoder, and a variational autoencoder. These neural networks are used to extract interaction parameters not only from neutron scattering length density profiles constructed using self-consistent field theory-based simulations, but also from a noisy ad hoc model constructed previously. In particular, the variational autoencoder is shown to be the most promising tool when it comes to the reconstruction and extraction of parameters from an ad hoc neutron scattering length density profile of a thin film containing a symmetric di-block copolymer (poly(deuterated styrene-b-n-butyl methacrylate)). This work paves the way for automated analysis of specular neutron reflectivities from thin films of copolymers using machine learning tools.

- **Publications:** All FY23 Q1 and Q2 CNMS publications for categories (publication types) (a) *Sole NSRC-led*, (b) *NSRC-led Collaborative*, (c) *NSRC/User Co-led Collaborative*, (d) *User-led Collaborative*, and (e) *User-only* are documented in the Excel spreadsheet (separate document "CNMS Publications FY23_Q1_Q2"). In Q1 (updated), CNMS had 61 publications with 34 publications in journals with an IF > 7 (56%) and in Q2, CNMS had 78 publications with 37 publications in journals with IF > 7 (47%).
- **Invention disclosures, patents, other products:**
  - None to report

**13. FWP Budget details**

- Budget information included in Excel spreadsheet (separate document " FY23 ORNL CNMS Budget_Q2").