

# NSRC Operations: Quarterly Report

**NSRC Name, DOE Laboratory(s):** Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory (ORNL)

**NSRC Director, Deputy:** Karren More, CNMS Director

**Date:** April 7, 2022

**Period covered:** January 1 to March 31, 2022

## 1. User Program:

### • User Updates

- **User Project Extensions:** We completed the review of extension requests for year-old projects due to expire at the end of January 2022. Forty-six applications for extension were approved for an additional year.
- **Proposal Call:** Spring Proposal Call opened in March with a proposal submittal deadline of May 4, 2022.
- **User Meeting Planning:** The CNMS User Executive Committees (UEC) asked CNMS staff to nominate potential speakers for this year's user meeting, which is scheduled for August 8-11, 2022. Staff also had the opportunity to suggest panel discussion themes, topics, and workshop ideas. The UEC plans to finalize the agenda and start inviting speakers in April.

### • Active User Projects

- Active User Proposals: 693
  - Industry-led: 19
  - University-led: 467
  - ORNL Staff-led: 164
  - Other Government Laboratory-led: 43
  - MSI and HBCU-led: 22
- Unique Institutions: 306
  - MSIs and HBCUs: 18
- Average User Time: 3.5 days
- Science Categories: User distribution - 60% Materials Science; 12% Engineering; 8% Chemistry; 5% Instrumentation; 4% Polymers; 4% Biological/Life Sciences; 3% Physics; 3% Optics; 2% 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): 84
  - R&D Staff: 63
  - Tech Professional: 5
  - Technician: 6
  - User Office: 2
  - Administrative: 6 (5 are supported at directorate level)
  - Operations (ES&H): 2 (both are supported at lab level)
- Total # FTEs supported on CNMS FWP (not including post-docs): 44.1
- Other funding sources/programs: 3 LDRD projects, 3 BES-MSED-FWPs, 1 SUFD-ECA, 1 CSGB-FWP, QSC, 3 EFRCS, multiple EERE offices (BETO, HFTO, VTO)

### • Changes

- **New Staff Hires:**

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Neus Domingo - Group Leader, Functional Atomic Force Microscopy Group; previously at the Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain

Saban Hus - R&D Associate, Scanning Tunneling Microscopy Group; previously at the University of Texas, Austin

Alexis Williams - R&D Associate, Materials MicroAnalysis Group; previously post-doc at Vanderbilt University

Honghai Zhang - R&D Associate, Macromolecular Nanomaterials Group; previously at Nanjing Technical University, China

Haoran Yu - Tech Professional in Materials MicroAnalysis Group; converted from CNMS post-doc

Biva Talukdar - Post-doc in Materials MicroAnalysis Group (BETO program); completed her PhD at Academia Sinica, Taiwan

John Villanova - Post-doc in Nanomaterials Theory Institute (QSC post-doc); previously post-doc at University of Arkansas

Hoyeon Jeon - Post-doc in Scanning Tunneling Microscopy Group (QSC post-doc); previously post-doc at Daegu Gyeongbuk Institute of Science and Technology, Korea

Annaberdiev Gani - Post-doc in Nanomaterials Theory Institute; Gani completed his PhD at North Carolina State University

Sang Yong Song - Post-doc in Functional Atomic Force Microscopy Group (MSED-FWP post-doc); previously at Daegu Gyeongbuk Institute of Science and Technology, Korea

## • Staff Departures:

Juan Carlos Idrobo - left for new position at University of Washington

Sergei Kalinin - left for a Principal Scientist position at Amazon for one year and will then join the University of Tennessee as the Weston Fulton Professor in the Materials Science and Engineering Department

(interviews for 2 group leader positions vacated by Juan (STEM) and Sergei (DNA) are underway)

Zhennan Huang - post-doc who took a new post-doc position at University of Maryland

## • Honors

Miaofang Chi was named a Microscopy Society of America (MSA) Fellow, Class of 2022.

Jordan Hachtel received two prestigious early career awards:

**2022 K.F.J. Heinrich Award** from the Microanalysis Society (MAS). This award recognizes Early Career Researchers with less than 15 years from their PhD who have made distinguished scientific and technical contributions to the field of microanalysis.

**2022 Albert Crewe Award** from the Microscopy Society of America (MSA), which is conferred for a single individual of not more than 6 years since PhD who has made distinguished contributions to the field of microscopy in the physical sciences.

Nikhil Sivasdas, a post-doc in the Nanomaterials Theory Institute, won the best postdoc presenter award at the international 'Ferro2022: Fundamental Physics of Ferroelectrics' Workshop for his talk titled "Anharmonic Stabilization of Ferrielectricity in Layered Thiophosphates: a First-Principles Case Study of  $\text{CuInP}_2\text{Se}_6$ " that is based on recent publication in *Physical Review Research* **4** 013094 (2022).

## • Significant Invited talks

Sergei V. Kalinin, "Physical Discovery in Automated Scanning Probe and Electron Microscopy," Computational Imaging Conference, Virtual, January 16-20, 2022.

Yongtao Liu, "Experimental Discovery of Structure-Property Relationships in Ferroelectric Materials via Active Learning," Electronic Materials and Applications 2022, Virtual, January 19-21, 2022.

Karren More, "Precision Synthesis at the Atomic Level," Additive Manufacturing Coalition Virtual Forum - Applications of Micro and Nano Scale 3D Printing in Medicine and Electronics, February 22, 2022.

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Jonathan Poplawsky, "Precipitate Strengthening and Stabilization Mechanisms in Cast and Additively Manufactured Al-Cu-Mn-Zr Alloys," TMS Annual Meeting, Virtual, February 27-March 3, 2022.

Rama Vasudevan, "Materials Physics from Microscopy: Statistical and Machine Learning Methods for Tackling Inverse Problems," APS March Meeting, Virtual, March 14-18, 2022.

Jordan Hachtel, "Nanoscale Analysis of Phonons, Polaritons, and Molecular Vibrations in Complex Materials," APS March Meeting, Chicago, IL, March 14-18, 2022.

Pat Collier, "Soft, Biologically Inspired Materials for Neuromorphic Memristors and Memcapacitors," ACS Spring Meeting, Virtual, March 20-24, 2022.

Kinga Unocic, "Investigation of Deactivation Mechanisms in Pt/TiO<sub>2</sub> Catalyst using Advanced and Operando STEM," ACS Spring Meeting, Virtual, March 20-24, 2022.

Miaofang Chi, "Probe Charge Transfer on the Sub-nm Scale in Heterogenous Catalysts via 4D-STEM," ACS Spring Meeting, San Diego, CA, March 20-24, 2022.

Miaofang Chi, "Atom-by-Atom Elucidation of Lattice Occupancy and Redox Dynamics of High Entropy Oxide (HEO) Catalysts," ACS Spring Meeting, San Diego, CA, March 20-24, 2022.

Kinga Unocic, "From *in situ* to *operando* Closed Cell Gas Reaction STEM: Challenges and Opportunities," In-situ/Operando TEM Techniques for Advanced Nanomaterial Characterization Workshop" hosted by McMaster University, Virtual, March 31 – April 1, 2022.

### 3. Postdocs Supported by FWP

- Total number of post-docs in CNMS Division: 27
- Number of post-docs supported by CNMS FWP: 12

### 4. Science Supported by FWP:

See Full List of Q2 Publications by Type at End of Report (pages 6-28).

### 5. Progress on BES NSRC-supported QIS FWP(s)

FWP ERKCZ62 "Precision Atomic Assembly for Quantum Information Science"

Lead PI - Arthur P. Baddorf

- All capital equipment budgeted for FY22 has been ordered.
  - Closed-cycle Low Temperature Scanning Tunneling Microscope (STM): This microscope is the heart of the project. After competitive evaluation the Infinity STM from Scienta Omicron was selected and ordered. Delivery expected in October 2022.
  - STM controller: Key to operation and interface to AI/ML algorithms. Competitive evaluation led to a Nanonis system from SPECS, which has been ordered. Delivery expected in June 2022.
- A laboratory for the STM has been identified, cleared, and is in the process of being prepared. Lab space is on the main campus (building 4515) and will be shared with mK-STM purchased as part of previous QIS Infrastructure project and is adjacent to lab housing the 4-probe STM. New electrical circuits have been installed. Other utilities (gas, water, exhaust) are being implemented. Engineering structures for liquid helium transfer lines to a compressor in a second room are being designed.
- The departure from ORNL of one of the co-investigators responsible for implementation of AI/ML (Sergei Kalinin) has been mitigated and work redistributed within the team.
- A CNMS User proposal has been written and accepted to explore atomic manipulation of individual metal atoms on metal substrates. Work has been initiated.

### 6. Progress on BES NSRC-supported ECRP FWP(s)

FWP ERKCZ55 "Probing Electrons in Electrified and Beyond"

Lead PI - Miaofang Chi

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- Work has focused on developing four-dimensional scanning transmission electron microscopy (4D-STEM) and atomic resolution cryogenic imaging. We successfully demonstrated imaging of light elements (i.e., Li and H) in materials using 4D-STEM, which has been challenging for conventional STEM. Atomic-resolution cryogenic STEM imaging at variable temperatures was realized by integrating a liquid nitrogen cooling stage with multi-frame acquisition followed by image registration and frame summing. By implementing atomic-scale cryogenic STEM imaging, phase transformations in  $\text{RuCl}_3$ , a Kitaev spin liquid candidate, were elucidated in real space. Results reconcile inconsistencies in previous studies that used reciprocal-space measurements.
- Future work on Electrides will focus on elucidating how anionic electron inhomogeneity in  $\text{Y}_5\text{Si}_3$  serves to tune its electronic structures. Forthcoming activities on van der Waals quantum materials will be to understand how phase transformation in  $\text{RuCl}_3$  influences interfacial charge transfer behavior in  $\text{RuCl}_3$ /graphene heterostructures.

## Publications:

- M. Zachman, Z. Yang, Y. Du, and M. Chi, "Robust Atomic-Resolution Imaging of Lithium in Battery Materials by Center-of-Mass Scanning Transmission Electron Microscopy," *ACS Nano* **16** (1) 1358-1367 (2022). DOI: 10.1021/acsnano.1c09374
- Y. Shi, R. Schimmenti, S. Zhu, K. Venkatraman, R. Chen, M. Chi, M. Shao, M. Mavrikakis, and Y. Xia, "Solution-Phase Synthesis of  $\text{Pd}_{0.706}$  Nanocubes with Enhanced Stability and Activity Toward Formic Acid Oxidation," *Journal of the American Chemical Society* **144** (6) 2556-2568 (2022). DOI: 10.1021/jacs.1c10199

## Invited Presentations:

- "Emerging Cryogenic and 4D-STEM for Quantum and Energy Materials," 6<sup>th</sup> Microscopy Characterization of Organic-Inorganic Interfaces (MCOII), Virtual, March 1-2, 2022.
- "Emerging Cryogenic and 4D-STEM for Quantum and Energy Materials," UCLA Department of Materials Science and Engineering Seminar, Virtual, February 11, 2022.
- "Probing Charge Transfer in Single Heterogeneous Catalysts via 4D-STEM," ACS Spring National Meeting, San Diego, CA, March 20-25, 2022.

## 7. 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
- FWP ERKCZ60 "A Collaborative Machine Learning Platform for Scientific Discovery" led by LBNL
- FWP ERKZZ61 "A Digital Twin for Spatiotemporally Resolved Experiments" led by ANL

## 8. Operations Equipment (EQU) Investments:

### • Replacement:

CNMS's original JEOL electron beam lithography (EBL) system was decommissioned and removed from the nanofabrication research laboratory. Site and facilities preparations were conducted prior to arrival of the new JEOL JBX-8100FS EBL instrument. Successful installation, power-up, and NRTL safety certification were completed by the last week of Q2. The first lithographic patterns have been written and are being qualified by JEOL. The first 3-4 weeks of Q3 will see NRL staff training completed with the tool fully operational and ready for users by week 5.

### • New:

CNMS acquired a fully automated large scanning AFM (DriveAFM, Nanosurf) equipped with hollow microfluidic probes for dispensing or aspirating down to femtoliter volumes of liquid. To date, Fluidic Force Microscopy (FluidFM) has been predominately used as a tool in life sciences for studying and controlling single cell function and dynamics. By incorporating automated positioning, microfluidic, and

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electrochemical control we will adapt FluidFM for a first of its kind platform for understanding applications in energy science, particularly related to catalysis.

## 8. Covid Impact

- Vaccinated users have been permitted to return to work onsite since mid-October 2021 in limited numbers
- In March 2022, all users (regardless of vaccination status) could return to campus with no limitations on the number of users working onsite at the same time
- Remote user work is still being conducted although users are being encouraged to work onsite
- All masking restrictions have been lifted for staff and visitors
- All CNMS (and ORNL) staff are expected to return to onsite work full-time by May 16, 2022 (most are already working onsite full time at CNMS)

## 9. Safety Updates

None to report

## 10. Concerns and Challenges

None to report

## 11. Other news

- P. Ganesh organized the 33<sup>rd</sup> Annual International Ferroelectrics Workshop: Ferro2022 - Fundamental Physics of Ferroelectrics, Virtual, February 6-9, 2022.
- A film crew worked at ORNL to produce a video "Atomic Manipulation for Quantum Materials at the CNMS" that highlighted CNMS staff and capabilities. Video will be featured at the APS Spring Meeting in Chicago, IL, March 14-18, 2022.
- Karren More served on the Peer Review Committee for the Nanotechnology Research Center (NANO), National Research Council, Canada, February 2022.
- Dr. Vanessa Chan, Chief Commercialization Officer and Director of the Office of Technology Transitions, U.S. Department of Energy toured the 3D Polymer Printing labs and cleanroom at CNMS on March 18, 2022.

## 12. Budget details

Budget information included as a separate attachment.

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## Center for Nanophase Materials Sciences (CNMS)

### Q2 Publication List

#### Publication Summary:

Total Number of Publications in Q2: 83

% Publications in High-Impact Journals (IF>7) in Q2: 53% (44/83)

#### Publication Type (a) - Sole CNMS Publications

Sivadas, N.; Doak, P.; Ganesh, P., "Anharmonic Stabilization of Ferrielectricity in  $\text{CuInP}_2\text{Se}_6$ ," *Physical Review Research* **4** (1) 013094 (2022). IF=too early

DOI: 10.1103/PhysRevResearch.4.013094

This research was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a DOE Office of Science User Facility and used resources of the Compute and Data Environment for Science (CADES) at ORNL. Computations also used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231. We thank Petro Maksymovych for discussions.

#### Publication Type (b) - CNMS-led Collaborative Publications

Buensuceso, C.E.; Tiu, B.D.B.; Lee, L.P.; Sabido, P.M.G.; Nuesca, G.M.; Caldonga, E.B.; del Mundo, E.B.; Advincula, R.C., "Electropolymerized-Molecularly Imprinted Polymers (E-MIPS) as Sensing Elements for the Detection of Dengue Infection," *Analytical and Bioanalytical Chemistry* **414** 1347-1357 (2022).

IF=3.286

DOI: 10.1007/s00216-021-03757-y

Work (or part of this work) was conducted by ORNL's Center for Nanophase Materials Sciences by RCA, which is a US Department of Energy Office of Science User Facility. The authors would like to express their gratitude to the following departments: Department of Macromolecular Science and Engineering—Case Western Reserve University, Institute of Chemistry—University of the Philippines (Diliman Campus), Park AFM Systems, and Biolin Scientific.

Burns, S.R.; Tselev, A.; Ievlev, A.V.; Agar, J.C.; Martin, L.W.; Kalinin, S.V.; Sando, D.; Maksymovych, P., "Tunable Microwave Conductance of Nanodomains in Ferroelectric  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  Thin Film," *Advanced Electronic Materials* **8** (3) 2100952 (2022). IF=7.295

DOI: 10.1002/aelm.202100952

Experiments and modelling have been carried out at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, which is a DOE Office of Science User Facility. This research was supported in part by the Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies (Project No. CE170100039) and funded by the Australian Government. This project was supported in part by an appointment to the Science Education and Workforce Development Programs at Oak Ridge National Laboratory, administered by ORISE through the U.S. Department of Energy Oak Ridge Institute for Science and Education. S.R.B. acknowledges funding in part from the UNSW Science Ph.D. Writing Scholarship and current funding from the Canada First Research Excellence Fund. In part (A.T.), this work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 and UIDP/50011/2020, financed by national funds through the FCT/MEC and when appropriate cofinanced by FEDER under the PT2020 Partnership Agreement.

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Creange, N.; Dyck, O.; Vasudevan, R.K.; Ziatdinov, M.; Kalinin, S.V., "Towards Automating Structural Discovery in Scanning Transmission Electron Microscopy," *Machine Learning Science & Technology* **3** (1) 015024 (2022). IF=2.940

DOI: 10.1088/2632-2153/ac3844

This effort (ML and STEM) is based upon work supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division (OD, SVK) and was performed and partially supported (RVK, MZ) at the Oak Ridge National Laboratory's Center for Nanophase Materials Sciences (CNMS), a U.S. Department of Energy, Office of Science User Facility. We thank Jacob Swett for preparing and providing the graphene sample, Wenrui Zhang and Gyula Eres for the preparation and providing the NiO-LSMO sample, Matthew Chisholm for acquiring the NiO-LSMO STEM data, Ziaohang Zhang and Ichiro Takeuchi for preparing and providing the Sm-BFO sample and Chris Nelson for acquiring the Sm-BFO STEM data.

da Silva, I.G.M.; Lucas, E.F.; Advincula, R., "Highly Efficient Oil/Water and Brine Separations: Superhydrophobic Hybrid Isobornyl Methacrylate Coatings," *Separation and Purification Technology* **278** 119365 (2022). IF=7.312

DOI: 10.1016/j.seppur.2021.119365

This study was supported in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001. Elizabete Lucas thanks FAPERJ (E-26/202.822/2017) and CNPq (303583/2019-3). We would like to thank Dr. Ina Martin (MORE Center at CWRU) for the profilometer measurements. Work (or Part of this work) was conducted by ORNL's Center for Nanophase Materials Sciences (R.C.Advincula), which is a US Department of Energy Office of Science User Facility.

de Souza, L.R.; d'Almeida, J.R.M.; Cheng, X.; Rong, L.; Caldona, E.B.; Advincula, R.C., "Highly Thermally Stable Copolymers of Epoxy and Trifunctional Polybenzoxazine," *Materials Today Communications* **30** 102988 (2022). IF=3.383

DOI: 10.1016/j.mtcomm.2021.102988

This work was supported by Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Brasil – Finance Code 001 for Lucio Souza. RC Advincula gratefully acknowledge funding from the Governor's Chair Funds, University of Tennessee system. Technical support from Malvern Panalytical, Frontier Laboratories and Quantum Analytics. Work (or Part of this work) was conducted by RC Advincula with the ORNL's Center for Nanophase Materials Sciences, which is a US Department of Energy Office of Science User Facility.

Hu, B.; Carrillo, J-M.; Collins, L.; Silmore, K.S.; Keum, J.; Bonnesen, P.V.; Wang, Y.; Retterer, S.; Kumar, R.; Lokitz, B.S., "Modular Approach for the Synthesis of Bottlebrush Diblock Copolymers from Poly(Glycidyl Methacrylate)-block-Poly(Vinylidimethylazlactone) Backbones," *Macromolecules* **55** (2) 488-497 (2022). IF=5.985

DOI: 10.1021/acs.macromol.1c01849

This research was conducted at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, which is a U.S. Department of Energy, Office of Science User Facility. Oak Ridge National Laboratory is operated for DOE Office of Science by UT Battelle, LLC, under contract number DE-AC05-00OR22725. K.S.S. was supported by the Department of Energy Computational Science Graduate Fellowship program under grant DE-FG02-97ER25308.

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Kalinin, S.V.; Steffes, J.J.; Liu, Y.; Huey, B.D.; Ziatdinov, M., "Disentangling Ferroelectric Domain Wall Geometries and Pathways in Dynamic Piezoresponse Force Microscopy via Unsupervised Machine Learning," *Nanotechnology* **33** (5) 055707 (2022). IF=3.874

DOI: 10.1088/1361-6528/ac2f5b

This research was conducted at the Center for Nanophase Materials Sciences, which also provided support (SVK, MZ) and is a US DOE Office of Science User Facility. The work was partially (YL) supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences Energy Frontier Research Centers program under Award Number DE-SC0021118. JJS and BDH recognize support from the NSF (MRI development award, DMR-1726862). The authors gratefully acknowledge R Ramesh (UC Berkeley) for the materials used in this study.

Liu, Z.; Lin, L.; Li, T.; Kinnun, J.; Hong, K.; Ma, Y-Z.; Sacci, R.L.; Katsaras, J.; Carrillo, J-M.; Doughty, B.; Collier, C. P., "Squeezing Out Interfacial Solvation: The Role of Hydrogen-Bonding in the Structural and Orientational Freedom of Molecular Self-Assembly," *Journal of Physical Chemistry Letters* **13** 2273-2280 (2022). IF=6.475

DOI: 10.1021/acs.jpcclett.1c03941

ODMS-MIM+ oligomer synthesis, molecular dynamics calculations, and manuscript preparation were performed at the Center for Nanophase Materials Sciences, which is a U.S. DOE Office of Science User Facility. SFG measurements and analysis, and manuscript preparation were supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, and Materials Sciences and Engineering Division. A portion of this research used resources at the Spallation Neutron Source, a U.S. DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. This research used resources of the Oak Ridge Leadership Computing Facility, which is a U.S. DOE Office of Science User Facility.

Lupke, F.; Pham, A.D.; Zhao, Y-F.; Zhou, L-J.; Lu, W.; Briggs, E.; Bernholc, J.; Kolmer, M.; Teeter, J.; Ko, W.; Zhang, C-Z.; Ganesh, P.; Li, A-P., "Local Manifestations of Thickness-Dependent Topology and Edge States in the Topological Magnet  $\text{MnBi}_2\text{Te}_4$ ," *Physical Review B* **105** (3) 035423 (2022). IF=4.036

DOI: 10.1103/PhysRevB.105.035423

This research was conducted at the Center for Nanophase Materials Sciences, which is a Department of Energy (DOE) Office of Science User Facility. F.L. acknowledges funding from the Alexander von Humboldt foundation through a Feodor Lynen postdoctoral fellowship. A.D.P.'s initial calculations were financially supported by the Oak Ridge National Laboratory's Laboratory Directed Research and Development project (Project ID No.7448, PI: P.G.). Subsequent computations by A.D.P. were supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as part of the Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials. The vasp calculations used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. DOE Office of Science User Facility operated under Contract No. DE-AC02-05CH11231. All computations using wannier90 code used resources of the Computer and Data Environment for Science (CADES) at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. DOE under Contract No. DE-AC05-00OR22725. The development of RMG was funded by the DOE Exascale Computing Project and the National Science Foundation Grant No. OAC-1740309. RMG based computations used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. DOE under Contract No. DE-AC05-00OR22725. The film growth done at Penn State is supported by the Gordon and Betty Moore Foundation's EPIQS Initiative (Grant No. GBMF9063 to C.Z.C.) and ARO Young Investigator Program Award (W911NF1810198). A portion of the research (A.-P.L.) is supported by the U.S. DOE, Office of Science, National Quantum Information Science Research Centers.

Mu, S.; Dixit, K.D.; Wang, X.; Abernathy, D.L.; Cao, H.; Nagler, S.E.; Yan, J.; Lampen-Kelley, P.; Mandrus, D.; Polanco, C.A.; Liang, L.; Halasz, G, B.; Cheng, Y.; Banerjee, A.; Berlijn, T., "Role of the Third



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Dimension in Searching for Majorana Fermions in  $\alpha$ -RuCl<sub>3</sub> via Phonons," *Physical Review Research* **4** 013067 (2022). IF=too new

DOI: 10.1103/PhysRevResearch.4.013067

The authors are grateful to Satoshi Okamoto, Pontus Laurell, Mengxing Ye, Simon Th ebaud, Peter Czjaka, and Lucas Lindsay for fruitful discussions and to Zach Morgan for his help with the extraction of the diffraction data. The work by T.B. was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility. The work by A.B., K.D., S.E.N., and G.B.H. has been supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Quantum Science Center. The work by S.M. and J.Y. was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. K.D. was also supported by Purdue University, College of Science, Ralf Scharenberg Fellowship. D.M. acknowledges support from the Gordon and Betty Moore Foundation's EPiQS Initiative, Grant Number GBMF9069. A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

Rong, L-H.; Cheng, X.; Ge, J.; Caldon, E.B.; Advincula, R.C., "Synthesis of Hyperbranched Polymers via PET-RAFT Self-Condensing Vinyl Polymerization in a Flow Reactor," *Macromolecular Chemistry and Physics* **223** (1) 2100342 (2022). IF=2.527

DOI: 10.1002/macp.202100342

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Vasudevan, R.K.; Ghosh, A.; Ziatdinov, M.; Kalinin, S.V., "Exploring Electron Beam Induced Atomic Assembly via Reinforcement Learning in a Molecular Dynamics Environment," *Nanotechnology* **33** (11) 115301 (2022). IF=3.874

DOI: 10.1088/1361-6528/ac394a

This effort was performed and partially supported (RKV, MZ) at the Oak Ridge National Laboratory's Center for Nanophase Materials Sciences (CNMS), a US Department of Energy, Office of Science User Facility, and by US Department of Energy, Office of Science, Office of Basic Energy Sciences Data, Artificial Intelligence and Machine Learning at DOE Scientific User Facilities program under Award Number 34532 (AG, SVK).

Zachman, M.J.; Yang, Z.; Du, Y.; Chi, M., "Robust Atomic-Resolution Imaging of Lithium in Battery Materials by Center-of-Mass Scanning Transmission Electron Microscopy," *ACS Nano* **16** (1) 1358-1367 (2022). IF=15.88

DOI: 10.1021/acsnano.1c09374

Work supported by DOE Basic Energy Sciences early career award ERKCZ55. The experimental and simulated electron microscopy was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility. M.C. was supported by DOE Basic Energy Sciences early career award ERKCZ55 and M.J.Z. by the Center for Nanophase Materials Sciences, a DOE Office of Science User Facility at Oak Ridge National Laboratory. LiCoO<sub>2</sub> thin film growth by Z.Y. and Y.D. was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES), Early Career Research Program under award number 68278.

## Publication Type (c) Collaborative Publications

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Aufrecht, J.A.; Khalid, M.; Walton, C. L.; Tate, K.; Cahill, J.F.; Retterer, S.T., "Hotspots of Root-Exuded Amino Acids are Created within a Rhizosphere-On-A-Chip," *Lab on a Chip* **22** (5) 954-963 (2022).

IF=6.799

DOI: 10.1039/d1lc00705j

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Wang, K.; Zhang, L.; Nguyen, G.D.; Sang, X.; Liu, C.; Yu, Y.; Ko, W.; Unocic, R.R.; Poretzky, A.A.; Rouleau, C.M.; Geohegan, D.B.; Fu, L.; Duscher, G.; Li, A-P.; Yoon, M.; Xiao, K., "Selective Antisite Defect Formation in WS<sub>2</sub> Monolayers via Reactive Growth on Dilute W-Au Alloy Substrates," *Advanced Materials* **34** (3) 2106674 (2022). IF=30.85

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