DEBANGSHU MUKHERJEE

R&D Associate Scientist,
Computational Chemistry and Nanomaterials Sciences Group,
Advanced Computing Methods for Physical Sciences Section,
Computational Sciences & Engineering Division,
Oak Ridge National Laboratory

mukherjeed@ornl.gov
1 Bethel Valley Rd, Oak Ridge, TN 37831-6057
(865) 341-1680 (Office) / (617) 501-7316 (Cell)
Links: ORNL Staff Website | Google Scholar |
ORNL Internal GitHub | Public Github |
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Research Interests

Coupling electron microscopy with High-Performance Computing	Designing the infrastructure to link HPC clusters with microscopes to analyze large datasets for rapid strain mapping, ptychography, real-time in-situ data analysis and automated microscope operations.
Quantitative electron imaging of quantum & energy materials	AI guided experiment design for structural and chemical understanding of interfaces/defects/surfaces in beam-sensitive material systems, such as quantum and energy materials.

Education

The Pennsylvania State University — *6/2013 — 5/2018*
Ph.D. in Materials Science & Engineering
Thesis advisor(s): Prof. Nasim Alem & Prof. Venkatraman Gopalan
Thesis title: Metrology of Ferroelectric Domain Walls with Scanning Transmission Electron Microscopy

Boston University — *8/2011 — 5/2013*
M.S. in Materials Science & Engineering
Thesis advisor(s): Prof. Soumendra Basu & Prof. Siddharth Ramachandran
Thesis title: Structured Semiconductor Fibers for Mid-Infrared Transmission

Indian Institute of Technology Kharagpur — *7/2006 — 5/2011*
B.Tech.(hons.), Metallurgical & Materials Engineering
M.Tech., Metallurgical Engineering
Thesis advisor(s): Prof. Sanat Kumar Roy & Prof. Shanker Ram
Thesis title: Synthesis and characterization of $La_{0.66}Ca_{0.33}MnO_3$ nanowires

Professional Experience

- Staff Scientist (R&D Associate)
  Computational Sciences & Engineering Division, Oak Ridge National Laboratory
  06/2021 – Present
- Postdoctoral Research Associate,
  Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
  06/2018 – 04/2021

Awards and Honors

- MAS Postdoctoral Scholar Award, 2020
- Dean's Fellowship, Boston University, 2011
- Best Bachelor's Thesis Award, IIT Kharagpur, 2010

Journal Publications, Book Chapters & Refereed Proceedings

In reverse chronological order

26. Al-Najjar A., Rao N.S.V., Sankaran R., Ziatdinov M.A., **Mukherjee, D.**, Roccapriore K.M., and Kalinin S.V.; Design-to-Deployment Continuum Platform for Microscopes and Computing Ecosystems. Accepted in *IEEE Transactions on Industrial Informatics*

25. Ul-Haque M.I., Lebron A., Alvarez F.J.D., Neal J.F., Mamak M., **Mukherjee, D.**, Ovchinnikova O.S., and Hinkle J.D.; Deep learning-driven super-resolution in Raman hyperspectral imaging: Efficient high-resolution reconstruction from low-resolution data. *Appl. Phys. Lett.* **125**, 204104 (2024)

24. Knight K., Danciu I., Ovchinnikova O., Hinkle J.D., Chandra Shekar M.C., **Mukherjee, D.**, McAllister E., Rizy C., Cho K., Justice A.C., Erdos J., Kuzmak P., Costa L., Ho Y-L., Madipadga R., Tamang S., Ian Goethert I.; VISION: Toward a Standardized Process for Radiology Image Management at the National Level *(Under Review)* arXiv:2404.18842

23. Kalinin, S.V., **Mukherjee, D.**, Roccapriore, K.M., Blaiszik, B., Ghosh, A., Ziatdinov, M.A., Al-Najjar, A., Doty, C., Akers, S., Rao, N.S. & Agar, J.C.; Machine learning for automated experimentation in scanning transmission electron microscopy *npj Computational Materials* **9**, 227 (2023) (Joint First and Corresponding Author)

22. Spurgeon, S.R., **Mukherjee, D.**, Gibson, W.S., Yang, S. & Lupini, A.R.; Focused Interest Groups Propel Innovation in the Emerging Data-Driven Hardware Ecosystem. *Microscopy Today* **31**(4), 20-21 (2023)

21. Al-Najjar, A., Rao, N.S., Sankaran, R., Zandi, H., **Mukherjee, D.**, Ziatdinov, M. and Bridges, C.; Cyber Framework for Steering and Measurements Collection Over Instrument-Computing Ecosystems. 2023 IEEE International Conference on Smart Computing (SMARTCOMP) 198-200, (2023)

20. Hinkle J.D. & **Mukherjee D.**; Interlaced scan patterns based on progressive hexagonal grids *(Under Review)* arXiv:2212.03356

19. Ul-Haque M.I., **Mukherjee D.**, Stopka S.A., Agar N.Y.R., Hinkle J.D. & Ovchinnikova O.S.; Deep Learning on Multimodal Chemical and Whole Slide Imaging Data for Predicting Prostate Cancer Directly from Tissue Images *J. Am. Soc. Mass Spectrom* **34**(2): 227 - 235 (023)

18. Rao N.S.V., Al-Najjar A., Zandi H., Sankaran R., Hicks S., Roccapriore K.M. & **Mukherjee D.**; Virtual Infrastructure Twins: Software Testing Platforms for Computing-Instrument Ecosystems *in Accelerating Science and Engineering Discoveries Through Integrated Research Infrastructure for Experiment, Big Data, Modeling and Simulation* Forthcoming Book Chapter

17. **Mukherjee D.**, Roccapriore K.M., Al-Najjar A., Ghosh A., Hinkle J.D., Lupini A.R., Vasudevan R.K., Kalinin S.V., Ovchinnikova O.S., Ziatdinov M.A. & Rao N.S.V.; A roadmap for edge computing enabled automated multidimensional transmission electron microscopy *Microscopy Today* **30**(6): 10 - 19 (2022)

16. Al-Najjar A., Rao N.S.V., Sankaran R., Ziatdinov M.A., **Mukherjee D.**, Ovchinnikova O.S., Roccapriore K.M., Lupini A.R. & Kalinin S.V.; Enabling Autonomous Electron Microscopy for Networked Computation and Steering *IEEE 18th International Conference on e-Science (e-Science)* (2022)

15. Miao L., Hasin K.-E., Moradifar P., **Mukherjee D.**, Ke Wang W., Cheong S.-W., Nowadnick E. & Alem N.; Double-Bilayer Polar Nanoregions and Mn antisites in $(Ca, Sr)_3Mn_2O_7$ *Nature Communications* **13**:4927 (2022)

14. Wang X., Tsaris A., **Mukherjee D.**, Wahib M., Chen P., Oxley M.P., Ovchinnikova O.S. & Hinkle J.D.; Image Gradient Decomposition for Parallel and Memory-Efficient Ptychographic Reconstruction. *SC' 22: Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis* (2022)

13. Miao L., Chmielewsk A., **Mukherjee D.** & Alem N.; Picometer-precision atomic position tracking through electron microscopy. *Journal of Visualized Experiments*, **173**:e62164 (2021)

12. Rimal G., Liu Y., Schmidt C., Hijazi H., Skoropata E., Lapano J.M., **Mukherjee D.**, Unocic R.R., Sun Y., Brahlek M., Feldman L.C, Ramanathan S. & Oh S.; Effective reduction of $PdCoO_2$ thin films via hydrogenation and sign tunable anomalous Hall effect. *Physical Review Materials*, **5**(5):L052001 (2021)

11. Zhang W., Mazza A.R., Skoropata E., **Mukherjee D.**, Musico B.L., Zhang J., Keppens V., Zhang L., Kisslinger K., Stavitski E., Brahlek M., Freeland J.W., Lu P. & Ward T.Z.; Applying configurational complexity to the 2D Ruddlesden-Popper crystal structure. *ACS Nano* **14**(10):13030-13037 (2020)

10. Lapano J.M., Mazza A.R., Li H., **Mukherjee D.**, Skoropota E., Ok J-M., Miao H., Moore R.G., Ward T.Z., Eres G., Lee H-N & Brahlek M.; Strong spin-dephasing in a topological insulator- paramagnet heterostructure. *APL Materials* **8**(9):091113 (2020)
9. Zhou X., Chen L., Sterbinsky G.A., **Mukherjee D.**, Unocic R.R. & Tait S.L.; Pt-ligand Single-atom Catalysts: Tuning Activity by Oxide Support Defect Density. *Catalysis Science & Technology*, **10**(10):3353-3365 (2020)
8. **Mukherjee D.**, Gamler. J.T.L., Skrabalak S.E. & Unocic R.R.; Lattice Strain Measurement of Core@Shell Electrocatalysts with 4D Scanning Transmission Electron Microscopy Nanobeam Electron Diffraction. *ACS Catalysis* **10**(10):5529-5541 (2020)
7. **Mukherjee D.**, Miao L., Stone G. & Alem N.; mpfit: a robust method for fitting atomic resolution images with multiple Gaussian peaks. *Advanced Structural and Chemical Imaging* **6**(1) (2020)
6. Brahlek M., Rimal G., Ok J.M., **Mukherjee D.**, Mazza A.R., Lu Q., Lee H.N., Ward T.Z., Unocic R.R., Eres G., & Oh, S.; Growth of metallic delafossite $PdCoO_2$ by molecular beam epitaxy. *Physical Review Materials* **3**(9):093401 (2019)
5. **Mukherjee D.**, Prokhorenko S., Miao L., Wang K., Bousquet E., Gopalan V. & Alem N.; Atomic-scale measurement of polar entropy. *Physical Review B* **100**(10):104102 (2019)
4. Young J., Moon E.J., **Mukherjee D.**, Stone G., Gopalan V., Alem N., May S.J. & Rondinelli J.M.; Polar oxides without inversion symmetry through vacancy and chemical order. *Journal of the American Chemical Society* **139**(7):2833-2841 (2017)
3. Zhang H.T., Zhang L., **Mukherjee D.**, Zheng Y.X., Haislmaier R.C., Alem N. & Engel-Herbert R.; Wafer-scale growth of VO_2 thin films using a combinatorial approach. *Nature Communications* **6**:8475 (2015)
2. Azizi A., Eichfeld S., Geschwind G., Zhang K., Jiang B., **Mukherjee D.**, Hossain L., Piasecki A.F., Kabius B., Robinson J.A. & Alem N.; Freestanding van der Waals heterostructures of graphene and transition metal dichalcogenides. *ACS Nano* **9**(5):4882-4890 (2015)
1. Sahu R.K., **Mukherjee D.**, Tiwari J.P., Mishra T., Roy S.K. & Pathak L.C.; Influence of foreign Fe ions on wet chemical synthesis of Pt nanoparticle thin films at ambient temperature: in situ versus direct addition *Journal of Materials Chemistry* **19**(37):6810-6815 (2009)

Patents

1. Ovchinnikova, O.S., Hinkle, J.D., Haque, I. and **Mukherjee, D.**, UT Battelle LLC, 2024. Machine learning on multimodal chemical and whole slide imaging data for predicting cancer labels directly from tissue images. U.S. Patent Application 18/340,306.

Manuscripts in Preparation

2. **Mukherjee D.**, Hinkle J.D. & Roccapriore K.M.; *Lossless compression of 4D–STEM datasets through entropy coding*
1. **Mukherjee D.**, Yu H., Wang C., Hinkle J.D., Spendelow J., Cullen D.A. and Zachman M.J. *Visualizing strain across hundreds of catalyst nanoparticles with 4D-STEM*

Conference Presentations

17. *Visualizing the Amorphous to Crystalline Transition of Bismuth Selenide in the TEM* **Microscopy & Microanalysis**, July 28 - August 1, 2024, Cleveland, Ohio.
16. *Integrating High-Performance Computing with Electron Microscopy for Scientific Insights* **Microscopy & Microanalysis**, July 28 - August 1, 2024, Cleveland, Ohio.
15. *Seamless Communication Between High-Performance Computing System and Electron Microscopes for On-Demand Automated Data Transfer and Remote Control*; **Microscopy & Microanalysis**, July 31 - August 4, 2022, Portland, Oregon.
14. *Efficient Memory Storage and Linear Parallel Scaling for Large-Scale Electron Ptychography*; **Microscopy & Microanalysis**, July 31 - August 4, 2022, Portland, Oregon.

13. *Lossless Image Compression for 4D-STEM Datasets*; **Microscopy & Microanalysis**, July 31 - August 4, 2022, Portland, Oregon.
12. *Automated methods for improved characterization of alloy nanoparticle catalysts*; **Microscopy & Microanalysis**, August 1-5, 2021, Virtual Conference.
11. *Quantifying the projected unit cell size variation of off-axis PtCo catalyst nanoparticles through 4D-STEM*; **Microscopy & Microanalysis**, August 1-5, 2021, Virtual Conference.
10. *Building an edge computing infrastructure for rapid multi-dimensional electron microscopy*; **Microscopy & Microanalysis**, August 1-5, 2021, Virtual Conference.
9. *Oxygen Annealing Driven Structural Evolution in $PdCoO_2$ Films Through Electron Microscopy*; **Microscopy & Microanalysis**, August 2-6, 2020, Virtual Conference.
8. *Stemtools: An Open Source Python Toolkit for Analyzing Electron Microscopy Datasets*; **Microscopy & Microanalysis**, August 2-6, 2020, Virtual Conference. (**2020 MSA Postdoctoral Scholar Award**)
7. *4D-STEM Data Acquisition, Analytics and Functional Material Property Extraction*; Invited Talk at **Materials Science & Technology**, October 1-4, 2019, Portland, Oregon.
6. *Investigation of Strain in Core@Shell Electrocatalysts with ADF-STEM and 4D-STEM Scanning Nanodiffraction*; **Microscopy & Microanalysis**, August 4-8, 2019, Portland, Oregon.
5. *4D-STEM Differential Phase Contrast Microscopy Across Ferroelectric Domain Walls*; **Microscopy & Microanalysis**, August 5-9, 2018, Baltimore, Maryland.
4. *Statistical Measurement of Polar Displacements in Complex Oxides*; **Microscopy & Microanalysis**, August 6-10, 2017, St. Louis, Missouri.
3. *Aberration Corrected STEM imaging of ferroelectric domain walls in $Ca_3Ru_{2(1-x)}Ti_xO_7$*; **APS March Meeting**, March 13-17, 2017; New Orleans, Louisiana.
2. *Aberration Corrected STEM Imaging of Domain Walls in Congruent $LiNbO_3$*; **Microscopy & Microanalysis**, July 24-28, 2016; Columbus, Ohio.
1. *Aberration Corrected Scanning Transmission Electron Microscopy of (Ca, Sr)Fe_2O_5 Brownmillerite superlattices*; **APS March Meeting**, March 14-18, 2016; Baltimore, Maryland.

Invited Talks:

4. *Solving Inverse Problems in Electron Microscopy with Differentiable Programing* Electronic Imaging 2025, February, 2025 (upcoming)
3. *Breaking the Resolution-Field of View Impasse in Catalyst Characterization with 4D-STEM* ACerS Electronic Materials & Applications Conference, February, 2024
2. *4D STEM Data Acquisition, Analytics and Functional Material Property Extraction* MS&T Conference, September 30th, 2019
1. *Gigabytes of data, picometers of precision* Infosys Condensed Matter Seminar, Tata Institute of Fundamental Research, July 26th, 2021

Grant Support

ORNL LDRD: INTERSECT Initiative
$ 600,000 per year for 3 years
10/2021 - 9/2024

Automated microscopy: 4D STEM and physics discovery
Role: PI
This project aimed at connecting electron microscopes at CNMS with HPC systems at OLCF, for automated electron microscopy.

DOE BRaVE:
Realize Understanding to Accelerate Design, Discovery, and Manufacturing of Materials.
$ 3,000,000 per year for 3 years
10/2023 - Present

Structure-guided Design of Materials to Optimize the Abiotic-Biotic Material Interface
Role: co-I
My role in this project is to develop tools for inverse reconstructions of optical microscopy data (ptychography), and single particle analysis codes for cryo-EM.

ORNL LDRD: ARM Initiative
$ 400,000 per year for 2 years
10/2023 - Present

Multimodal analysis of Nuclear Medicine by cryoEM
Role: co-PI
My role here is developing AI based particle counting methods for noisy cryo-EM data.

ORNL LDRD: INTERSECT Initiative
$ 400,000 per year for 3 years
10/2023 - Present

Quantum Correlated Materials Accelerated Discovery Platform (Q-CAD)
Role: co-PI
My role here is building neural networks for quantifying materials change from the CBED patterns, as they evolve in-situ. Additionally, we are developing fully differentiable RHEED simulators for real-time inverse reconstructions of RHEED data as the material grows in the MBE.

Conference/Workshop Organization

- *New Opportunities in Material Science – Multi-dimensional Imaging and Advanced Data Processing* – 2024 M&M Conference.
- *Pre-Meeting Congress on Synergy of Hardware Innovations and Computational Breakthroughs in TEM* – 2024 M&M Conference as the Chair of EM-DAM FIG, jointly with the Aberration-Corrected FIG.
- *Pre-Meeting Congress on Software Developments in Microscopy* – At the 2023 M&M Conference as the Chair of Electron Microscopy Data Analysis & Management (EM-DAM) Focused Interest Group (FIG), jointly with Aberration-Corrected FIG
- *Computational Advances in Electron Microscopy* – Chaired the 2023 M&M Session
- *AI in STEM Workshop* – at the Oak Ridge National Laboratory, December, 2020

Skills

- Software development and data visualization in `python` and `MATLAB`
- High-performance computing on Summit and Frontier supercomputers.
- Mechanical and Focused Ion Beam Sample Preparation
- Operation of Thermo-Fisher (FEI), NION and JEOL aberration-corrected electron microscopy systems
- Chemical Vapor Deposition of 2D crystals (graphene, *h*-BN, MoS_2)

Teaching Experience

- Introduction to Materials Characterization *Fall 2016*
- Transmission Electron Microscopy *Fall 2015* — Penn State
- Crystal Chemistry *Fall 2013*

- Engineering Thermodynamics *Spring 2012* — Boston University

Mentoring Experience

Sai Venkata Gayathri Ayyagari
08/2024 – Present

PhD student from Penn State (Alem Group), working on structural quantification of high-entropy oxide thin films.

Gabriel A. Vázquez-Lizardi
06/2024 – Present

DOE SCGSR Intern from The Pennsylvania State University (Hickey Group). Gabriel is working on the development of a machine learning framework for automated electron microscopy data analysis.

Md. Inzamam Ul-Haque
2021 – 12/2023

University of Tennessee Bredesen center graduate student, *I was the thesis advisor for Inzamam.* Inzamam defended his thesis, and is working as ML engineer at ThermoFisher Scientific.

Leixin Miao
2016-2018

Mentored and taught TEM sample preparation through FIB, analysis of STEM datasets with MATLAB scripts, and microscope image simulation through MATLAB . Leixin continued as a PhD student with my doctoral advisor – Dr. Nasim Alem. He defended in October 2022, and is now a TEM Engineer at Intel, Portland, USA.