Debangshu **Mukherjee**

R&D Associate Scientist
Computational Sciences & Engineering Division
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Research Interests

Coupling electron microscopy with High-Performance Computing
Designing the infrastructure necessary to link leadership class high-performance compute clusters with microscopes. The aim is analysis of large datasets for rapid strain mapping, ptychography, real-time in-situ data analysis and automated microscope operations.

Design of experiments for quantitative electron imaging of quantum & energy materials
AI guided experiment design, for quantitative structural and chemical understanding of interfaces/defects/surfaces in beam-sensitive material systems, such as quantum and energy materials.

Education

The Pennsylvania State University
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
6/2013 — 5/2018

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

Indian Institute of Technology Kharagpur
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
7/2006 — 5/2011

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
- Graduate Research/Teaching Assistant
  Department of Materials Science & Engineering, The Pennsylvania State University
  06/2013 – 05/2018
- Graduate Research/Teaching Assistant
  Department of Materials Science & Engineering, Boston University
  08/2011 – 05/2013

Awards and Honors

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

Publications

20. Hinkle J.D. & **Mukherjee D.**; Interlaced scan patterns based on progressive hexagonal grids *(Under Review)* arXiv:2212.03356 (2022)

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 *Accepted in Journal of the American Society for Mass Spectrometry* bioRxiv 2022.05.11.491570

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)

Manuscripts in Preparation

4. **Mukherjee D.**, Hinkle J.D. & Roccapriore K.M.; *Lossless compression of 4D–STEM datasets through entropy coding*

3. **Mukherjee D.**, Yu H., Spendelow J., Cullen D.A. and Zachman M.J. *Visualizing strain across hundreds of catalyst nanoparticles with 4D-STEM*

2. **Mukherjee D.**, Lapano J.L., Rimal G., Lee H.N. and Brahlek M. *Effect of oxygen annealing on the $PdCoO_2$ film - Al_2O_3 substrate interface*

1. **Mukherjee D.** and Unocic R.R. *STEMTool: A Python based open source software suite for scanning transmission electron microscopy data analysis*

Conference Presentations

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:

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: Automated microscopy: 4D STEM and physics discovery
2021 - Present Role: co-PI

Skills

- Software development and data visualization in `python` and `MATLAB`
- Distributed Python programming with `dask`
- GPU programming in Python with `cupy`
- Machine learning with `pytorch` and `JAX`
- 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

Md. Inzamam Ul-Haque
2021-Present
University of Tennessee Bredesen center graduate student, *currently I am the main thesis advisor for Inzamam.*

Matthew Drexler
2018-2019
ORNL visiting graduate researcher from Georgia Tech, whom I mentored and taught STEM operation and data collection with the NION microscopes.

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.

Michael Brova
2014
Mentored and taught CVD growth of 2D crystals, and transfer of 2D materials onto TEM grids. Michael subsequently continued at Penn State for a PhD, and following his doctorate joined Intel as a process engineer.

References

Dr. Sergei Vasilyevich Kalinin
AmazonScience Faculty Fellow (till March 2023),
Weston Fulton Professor of Engineering (04/2023 –)
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