Debangshu **Mukherjee**

R&D Associate Scientist

Computational Sciences & Engineering Division

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Research Interests

Quantitative Electron Imaging of Quantum & Energy Materials	Quantitative structural and chemical understanding of interfaces/defects/surfaces in quantum and energy materials with high-precision electron microscopy, across multiple temperature regimes.
Coupling Electron Microscopy with HPC	Analysis of gigabyte-scale datasets on high-performance compute clusters for fast and high precision strain mapping, ptychography and automated microscope operation.

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

14. **Mukherjee D.**, Unocic R.R., Strain quantification of catalyst nanoparticles with 4D-STEM. Under review in *JoVE*

13. Miao L., Chmielewsk A., **Mukherjee D.**, Alem N., Picometer-precision atomic position tracking through electron microscopy. *Journal of Visualized Experiments*, e62164

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. and Oh S., Effective reduction of $PdCoO_2$ thin films via hydrogenation and sign tunable anomalous Hall effect. *Physical Review Materials*, 5(5):L052001

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. and Ward T.Z., Applying configurational complexity to the 2D Ruddlesden-Popper crystal structure. *ACS Nano* 14(10):13030-13037

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 and Brahlek M, Strong spin-dephasing in a topological insulator- paramagnet heterostructure. *APL Materials* 8(9):091113

9. Zhou X., Chen L., Sterbinsky G.A., **Mukherjee D.**, Unocic R.R. and Tait S.L.; Pt-ligand Single-atom Catalysts: Tuning Activity by Oxide Support Defect Density. *Catalysis Science & Technology*, 10(10):3353-3365

8. **Mukherjee D.**, Gamler. J.T.L., Skrabalak S.E. and 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

7. **Mukherjee D.**, Miao L., Stone G., and Alem N.; mpfit: a robust method for fitting atomic resolution images with multiple Gaussian peaks. *Advanced Structural and Chemical Imaging* 6(1)

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. and Oh, S.; Growth of metallic delafossite $PdCoO_2$ by molecular beam epitaxy. *Physical Review Materials* 3(9):093401

5. **Mukherjee D.**, Prokhorenko S., Miao L., Wang K., Bousquet E., Gopalan V. and Alem N.; Atomic-scale measurement of polar entropy. *Physical Review B* 100(10):104102

4. Young J., Moon E.J., **Mukherjee D.**, Stone G., Gopalan V., Alem N., May S.J. and Rondinelli J.M.; Polar oxides without inversion symmetry through vacancy and chemical order. *Journal of the American Chemical Society* 139(7):2833-2841

3. Zhang H.T., Zhang L., **Mukherjee D.**, Zheng Y.X., Haislmaier R.C., Alem N. and Engel-Herbert R.; Wafer-scale growth of VO_2 thin films using a combinatorial approach. *Nature Communications* 6:8475

2. Azizi A., Eichfeld S., Geschwind G., Zhang K., Jiang B., **Mukherjee D.**, Hossain L., Piasecki A.F., Kabius B., Robinson J.A. and Alem N; Freestanding van der Waals heterostructures of graphene and transition metal dichalcogenides. *ACS Nano* 9(5):4882-4890

1. Sahu R.K., **Mukherjee D.**, Tiwari J.P., Mishra T., Roy S.K. and 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

Manuscripts in Preparation

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

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.

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`
- 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 co-advising with Dr. Jacob Hinkle & Dr. Olga S. Ovchinnikova.

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.

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 V. Kalinin
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