

Debangshu Mukherjee

Materials science | Machine learning | Automated experiments

debangshu-mukherjee.com | contact@debangshu-mukherjee.com

GitHub: [debangshu-mukherjee](#) | [Google Scholar](#) | [LinkedIn](#)

Research profile

I build physical models and computational tools for understanding materials measurements. My experimental experience spans electron microscopy, optical microscopy, and RHEED measurements. I combine that hands-on work with inverse problems, GPU computing, and interfaces that let AI agents run simulation and reconstruction workflows.

Appointments

Staff Scientist (R&D Associate)

June 2021 – September 2026

Oak Ridge National Laboratory · Computational Sciences & Engineering Division

I connected electron microscopy with high-performance computing for quantitative imaging and automated experiments. I also coauthored work on machine learning for microscope workflows, distributed ptychographic reconstruction, and infrastructure for instrument control and data transfer.

Postdoctoral Research Associate

June 2018 – April 2021

Oak Ridge National Laboratory · Center for Nanophase Materials Sciences

I developed quantitative methods for extracting structure from microscopy data, including 4D-STEM strain mapping of core-shell catalysts and robust fitting of atomic positions in images.

Graduate Research / Teaching Assistant

June 2013 – May 2018

The Pennsylvania State University · Materials Science & Engineering

I studied ferroelectric domain walls using scanning transmission electron microscopy.

Graduate Research / Teaching Assistant

August 2011 – May 2013

Boston University · Materials Science & Engineering

I studied structured semiconductor fibers for mid-infrared transmission.

Education

Ph.D., Materials Science & Engineering

The Pennsylvania State University · 2013 – 2018

Thesis: Metrology of Ferroelectric Domain Walls with Scanning Transmission Electron Microscopy.

Advisors: Nasim Alem and Venkatraman Gopalan

M.S., Materials Science & Engineering

Boston University · 2011 – 2013

Thesis: Structured Semiconductor Fibers for Mid-Infrared Transmission.

Advisors: Soumendra Basu and Siddharth Ramachandran

B.Tech. (Honors), Metallurgical & Materials Engineering; M.Tech., Metallurgical Engineering

Indian Institute of Technology Kharagpur · 2006 – 2011

Thesis: Synthesis and characterization of $\text{La}_{0.66}\text{Ca}_{0.33}\text{MnO}_3$ nanowires.

Advisors: Sanat Kumar Roy and Shanker Ram

Selected research contributions

Experiments connected to computing

Coauthor

My collaborators and I investigated networked computation and steering for electron microscopy, connecting instrument control and data transfer with remote analysis. This work addresses the infrastructure needed for automated experiments.

Ptychographic reconstruction at scale

Coauthor; published team result

In our SC22 study, we reconstructed a PbTiO₃ dataset with 16,632 probe positions in 2.2 minutes on 4,158 GPUs using image gradient decomposition. The method distributes reconstruction while reducing memory requirements.

Quantitative materials characterization

First author

In our ACS Catalysis study, we used 4D-STEM to measure lattice strain in rhodium–platinum core–shell nanocubes with sub-picometer precision. The analysis resolves structural changes across the core–shell interface.

Technical skills

Machine learning & differentiable physics

I use JAX, PyTorch, automatic differentiation, and physical forward models to tackle inverse problems and learn from scientific imaging data. My work connects model fitting and data analysis with experimental workflows.

Scientific software & computing

I develop scientific software in Python and MATLAB, using JAX, Dask, CuPy, GPU computing, and distributed analysis. I built chatbot integrations that expose compiled simulation and reconstruction workflows to agents through discoverable task interfaces and structured results.

Microscopy, spectroscopy & materials

Hands-on electron microscopy, optical microscopy, and reflection high-energy electron diffraction (RHEED) measurements. Additional expertise includes angle-resolved photoemission spectroscopy (ARPES), 4D-STEM, ptychography, strain mapping, atomic-resolution image analysis, aberration-corrected electron microscopy (Thermo Fisher / FEI, NION, and JEOL), focused ion beam sample preparation, and chemical vapor deposition of 2D materials.

Open source scientific software

Janssen — differentiable wave optics and ptychographic phase retrieval

Composable wave propagation and optical elements; JAX PyTrees carry complex fields and coherence modes for simulation and phase retrieval.

[GitHub](#) | [Documentation](#)

Ptyrodactyl — differentiable electron scattering and reconstruction

Separate scattering models share validated physical data structures; array-based numerical kernels are separated from crystal parsing and file I/O.

[GitHub](#) | [Documentation](#)

Rheedium — crystal-to-diffraction simulation and parameter fitting

Crystal-to-detector forward models support constrained inverse problems; physical invariants and reference comparisons help validate the numerical results.

[GitHub](#) | [Documentation](#)

diffpes — electronic-structure-to-photoemission simulation in JAX

Electronic structure, photoemission, and instrument response are modeled separately; continuous parameters support differentiation, with explicit treatment of degeneracy and unidentifiable directions.

[GitHub](#) | [Documentation](#)

I built end-to-end RHEED and ARPES simulators with chatbot integrations through automatons. These expose ahead-of-time (AOT) compiled JAX workflows through discoverable task interfaces, enabling real-time simulation and reconstruction from a computer or phone during experiments. Agents inspect task descriptions and structured results instead of navigating the full scientific implementation.

Additional scientific software

CryoBlob

I built CryoBlob for reference-free detection of compact features in low-signal cryo-EM images, using JAX compilation and GPU acceleration.

[GitHub](#) | [Documentation](#)

stemtool

I built stemtool as an open source Python toolkit for analyzing scanning transmission electron microscopy datasets.

[GitHub](#) | [Documentation](#)

Awards and honors

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

Teaching

- Introduction to Materials Characterization — Penn State, Fall 2016
- Transmission Electron Microscopy — Penn State, Fall 2015
- Crystal Chemistry — Penn State, Fall 2013
- Engineering Thermodynamics — Boston University, Spring 2012

Mentoring

I have mentored graduate researchers in electron microscopy, data analysis, specimen preparation, and 2D materials growth, including Md. Inzamam Ul-Haque, Matthew Drexler, Leixin Miao, and Michael Brova.

Publications and scholarly contributions

Bibliography reviewed September 28, 2026. Duplicate entries are consolidated; distinct conference contributions, software releases, theses, and preprints are listed by type. Titles link to verified DOIs where available, or to original records. Author lists may be abbreviated.

Journal publication

1. [Error-Guaranteed Compression with Preservation of Downstream Quantities for Electron Microscopy](#)
J Lee, ER Hogle, Q Gong, AR Lupini, D Mukherjee, AN Williams, ...
Microscopy and Microanalysis 32 (4), 02084, 2026
2. [Evidence of Local Structural Variations and Their Influence on Magnetic Properties in Mn- and Cr-Containing High-Entropy Oxide Thin Films Using Electron Microscopy](#)
SVG Ayyagari, M Webb, JT Sivak, G Bejger, JP Barber, D Mukherjee, ...
Journal of the American Chemical Society 148 (22), 22521, 2026
3. [Intrinsic even-odd thickness-driven anomalous Hall effect in epitaxial MnBi₂Te₄ thin films](#)
D Mallick, S Kim, AH Chen, GA Vázquez-Lizardi, AR Mazza, TZ Ward, ...
Physical Review Materials 10 (4), 044203, 2026
4. [Nucleation and Antiphase Twin Control in Bi₂Se₃ via Step-Terminated Al₂O₃ Substrates](#)
AR Mazza, J Shi, GA Vázquez-Lizardi, S Kim, J Bentley, AH Chen, ...
Advanced Functional Materials 36 (22), e13054, 2026
5. [Design-to-deployment continuum platform for microscopes and computing ecosystems](#)
A Al-Najjar, NSV Rao, R Sankaran, D Mukherjee, K Roccapriore, ...
IEEE Transactions on Industrial Informatics 21 (5), 3645-3654, 2025
6. [Deep learning-driven super-resolution in Raman hyperspectral imaging: Efficient high-resolution reconstruction from low-resolution data](#)
MIU Haque, A Lebron, FJD Alvarez, JF Neal, M Mamak, D Mukherjee, ...
Applied Physics Letters 125, 204104, 2024

7. **Machine learning for automated experimentation in scanning transmission electron microscopy**
SV Kalinin, D Mukherjee, K Roccapriore, BJ Blaiszik, A Ghosh, ...
npj Computational Materials 9 (1), 227, 2023
8. **Focused Interest Groups Propel Innovation in the Emerging Data-Driven Hardware Ecosystem**
SR Spurgeon, D Mukherjee, WS Gibson, S Yang, AR Lupini
Microscopy Today 31 (4), 20-21, 2023
9. **Deep learning on multimodal chemical and whole slide imaging data for predicting prostate cancer directly from tissue images**
MIU Haque, D Mukherjee, SA Stopka, NYR Agar, J Hinkle, ...
Journal of the American Society for Mass Spectrometry 34 (2), 227, 2023
10. **A roadmap for edge computing enabled automated multidimensional transmission electron microscopy**
D Mukherjee, KM Roccapriore, A Al-Najjar, A Ghosh, JD Hinkle, ...
Microscopy Today 30 (6), 10-19, 2022
11. **Double-Bilayer Polar Nanoregions and Mn antisites in (Ca, Sr) $3\text{Mn}_2\text{O}_7$**
L Miao, KE Hasin, P Moradifar, D Mukherjee, K Wang, SW Cheong, ...
Nature Communications 13, 2022
12. **Picometer-precision atomic position tracking through electron microscopy**
L Miao, A Chmielewski, D Mukherjee, N Alem
JoVE (Journal of Visualized Experiments), e62164, 2021
13. **Effective reduction of PdCoO_2 thin films via hydrogenation and sign tunable anomalous Hall effect**
G Rimal, C Schmidt, H Hijazi, LC Feldman, Y Liu, E Skoropata, J Lapano, ...
Physical Review Materials 5 (5), L052001, 2021
14. **Strong spin-dephasing in a topological insulator-paramagnet heterostructure**
J Lapano, AR Mazza, H Li, D Mukherjee, EM Skoropata, JM Ok, H Miao, ...
APL Materials 8 (9), 091113, 2020
15. **Applying Configurational Complexity to the 2D Ruddlesden–Popper Crystal Structure**
W Zhang, AR Mazza, E Skoropata, D Mukherjee, BL Musico, J Zhang, ...
ACS Nano 14 (10), 13030-13037, 2020
16. **Pt-ligand Single-atom Catalysts: Tuning Activity by Oxide Support Defect Density**
X Zhou, L Chen, GE Sterbinsky, D Mukherjee, RR Unocic, SL Tait
Catalysis Science & Technology 10 (10), 3353-3365, 2020
17. **Lattice Strain Measurement of Core@Shell Electrocatalysts with 4D Scanning Transmission Electron Microscopy Nanobeam Electron Diffraction**
D Mukherjee, JTL Gamler, SE Skrabalak, RR Unocic
ACS Catalysis 10 (10), 5529-5541, 2020
18. **mpfit: a robust method for fitting atomic resolution images with multiple Gaussian peaks**
D Mukherjee, L Miao, G Stone, N Alem
Advanced Structural and Chemical Imaging 6 (1), 2020
19. **Growth of metallic delafossite PdCoO_2 by molecular beam epitaxy**
M Brahlek, G Rimal, JM Ok, D Mukherjee, AR Mazza, Q Lu, HN Lee, ...
Physical Review Materials 3 (9), 093401, 2019
20. **Atomic-scale measurement of polar entropy**
D Mukherjee, S Prokhorenko, L Miao, K Wang, E Bousquet, V Gopalan, ...
Physical Review B 100 (10), 104102, 2019
21. **Polar oxides without inversion symmetry through vacancy and chemical order**
J Young, EJ Moon, D Mukherjee, G Stone, V Gopalan, N Alem, SJ May, ...
Journal of the American Chemical Society 139 (7), 2833-2841, 2017
22. **Wafer-scale growth of VO_2 thin films using a combinatorial approach**
HT Zhang, L Zhang, D Mukherjee, YX Zheng, RC Haislmaier, N Alem, ...
Nature Communications 6 (8475), 2015

23. **Freestanding van der Waals Heterostructures of Graphene and Transition Metal Dichalcogenides**
A Azizi, SM Eichfeld, G Geschwind, K Zhang, B Jiang, D Mukherjee, ...
ACS Nano 9 (5), 4882-4890, 2015
24. **Influence of foreign Fe ions on wet chemical synthesis of Pt nanoparticle thin films at ambient temperature: in situ versus direct addition**
RK Sahu, D Mukherjee, JP Tiwari, T Mishra, SK Roy, LC Pathak
J. Mater. Chem. 19 (37), 6810-6815, 2009

Conference abstract

1. **Probing the Local Structure and Electronic States of Strained High Entropy Oxide Heterostructures**
SVG Ayyagari, SSI Almishal, D Mukherjee, KM Roccapriore, JP Maria, ...
Microscopy and Microanalysis 32 (Supplement_1), ozag053. 600, 2026
2. **Electron Ptychography via Differentiable Programming**
D Mukherjee, R Sankaran, MJ Boebinger
Microscopy and Microanalysis 31 (Supplement_1), ozaf048. 038, 2025
3. **Modular Optical Ptychography through Differentiable Programming**
D Mukherjee, MJ Blake, B Doughty
Microscopy and Microanalysis 31 (Supplement_1), ozaf048. 435, 2025
4. **Deciphering Growth Kinetics of a Topological Insulator using in-situ 4D-STEM**
MG Boebinger, D Mukherjee, Z Wu, J Chen, S Bagchi, M Brahlek, ...
Microscopy and Microanalysis 31 (Supplement_1), ozaf048. 092, 2025
5. **Visualizing the Amorphous to Crystalline Transition of Bismuth Selenide in the TEM**
D Mukherjee, JAH Chen, A Ghosh, S Bagchi, P Ganesh, MJ Brahlek, ...
Microscopy and Microanalysis 30 (Supplement_1), ozae044. 715, 2024
6. **Integrating high-performance computing with electron microscopy for scientific insights**
A Ghosh, K Roccapriore, MG Boebinger, D Mukherjee, A Al-Najjar, ...
Microscopy and Microanalysis 30 (Supplement_1), ozae044. 162, 2024
7. **Atomic Scale Structure of Ferroelectric Domain Walls**
G Stone, D Mukherjee, N Alem, V Gopalan
Microscopy and Microanalysis 30 (Supplement_1), ozae044. 527, 2024
8. **Lossless Image Compression for 4D-STEM Datasets**
J Hinkle, D Mukherjee, K Roccapriore, A Rakowski, C Nelson, O Dyck, ...
Microscopy and Microanalysis 28 (S1), 3060-3061, 2022
9. **Seamless communication between high-performance computing system and electron microscopes for on-demand automated data transfer and remote control**
D Mukherjee, A Al-Najjar, KM Roccapriore, JD Hinkle, AR Lupini, C Meyer, ...
Microscopy and Microanalysis 28 (S1), 2908-2910, 2022
10. **Efficient Memory Storage and Linear Parallel Scaling for Large-Scale Electron Ptychography**
X Wang, D Mukherjee, M Oxley, O Ovchinnikova, J Hinkle
Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States) 28 (S1), 2022
11. **Predicting Prostate Cancer Directly from Tissue Images using Deep Learning on Mass Spectrometry Imaging and Whole Slide Imaging Data**
MIU Haque, D Mukherjee, S Stopka, NYR Agar, J Hinkle, O Ovchinnikova
Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States) 28 (S1), 2022
12. **Direct observation of polar/non-polar phase coexistence in $\text{Ca}_{2.9}\text{Sr}_{0.1}\text{Mn}_2\text{O}_7$**
KE Hasin, E Nowadnick, L Miao, FT Huang, P Moradifar, D Mukherjee, ...
APS March Meeting Abstracts 2022, Y70. 006, 2022
13. **Mapping the Evolution of Surface Strain in PtCo Core-Shell Catalysts By 4D-STEM**
MJ Zachman, D Mukherjee, C Wang, H Yu, JS Spendelow, DA Cullen
Electrochemical Society Meeting Abstracts 240, 1020-1020, 2021

14. **Quantifying the projected unit cell size variation of off-axis PtCo catalyst nanoparticles through 4D-STEM**
D Mukherjee, H Yu, C Wang, J Spendelow, D Cullen, M Zachman
Microscopy and microanalysis 27 (S1), 1440-1442, 2021
15. **Building an edge computing infrastructure for rapid multi-dimensional electron microscopy**
D Bhowmik, D Mukherjee, M Oxley, M Ziatdinov, S Jesse, S Kalinin, ...
Microscopy and Microanalysis 27 (S1), 56-57, 2021
16. **Automated methods for improved characterization of alloy nanoparticle catalysts**
DA Cullen, M Zachman, H Yu, D Mukherjee, SK Reeves
Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States) 27 (S1), 2021
17. **Ferromagnetism and sign-tunable anomalous hall effect in PdCoO₂ via hydrogenation**
G Rimal, Y Liu, C Schmidt, H Hijazi, E Skoropata, J Lapano, D Mukherjee, ...
APS March Meeting Abstracts 2021, X36. 009, 2021
18. **Oxygen Annealing Driven Structural Evolution in PdCoO₂ Films Through Electron Microscopy**
D Mukherjee, G Rimal, RR Unocic, HN Lee, S Oh, M Brahlek
Microscopy and Microanalysis 26 (S2), 612-613, 2020
19. **Asymmetry and 4D-STEM: When the Phase Object Approximation Is Qualitatively Incorrect**
M Oxley, D Mukherjee, J Hachtel
Microscopy and Microanalysis 26 (S2), 1910-1911, 2020
20. **STEMTooL: An Open Source Python Toolkit for Analyzing Electron Microscopy Datasets**
D Mukherjee, RR Unocic
Microscopy and Microanalysis 26 (S2), 2960-2962, 2020
21. **High Resolution S/Transmission Electron Microscopy Investigation of Ca₃Mn₂O₇ Phase Transformation under In-situ Heating Condition**
L Miao, P Moradifar, D Mukherjee, R Hu, SW Cheong, N Alem
Microscopy and Microanalysis 25 (S2), 1876-1877, 2019
22. **Investigation of strain in core@ shell electrocatalysts with ADF-STEM and 4D STEM scanning nanodiffraction**
D Mukherjee
Microscopy and Microanalysis, 2019
23. **High Resolution S/TEM Imaging of High Density Domain Stacking and Coexisting Polar-nonpolar Phases in Layered Perovskite Ca₃Mn₂O₇**
L Miao, D Mukherjee, R Hu, SW Cheong, N Alem
Microscopy and Microanalysis 24 (S1), 1916-1917, 2018
24. **4D-STEM differential phase contrast microscopy across ferroelectric domain walls**
D Mukherjee, C Ophus, J Ciston, Z Mao, V Gopalan, N Alem, PA Park
Microsc. Microanal 24, 228-229, 2018
25. **Statistical Measurement of Polar Displacements in Complex Oxides**
L Miao, D Mukherjee, G Stone, N Alem
Microscopy and Microanalysis 23 (S1), 1660-1661, 2017
26. **Aberration Corrected STEM imaging of ferroelectric domain walls in Ca₃Ru₂(1-x)Ti_xO₇**
D Mukherjee, S Lei, Z Mao, V Gopalan, N Alem
Bulletin of the American Physical Society 62 (4), 2017
27. **Aberration Corrected STEM Imaging of Domain Walls in Congruent LiNbO₃**
D Mukherjee, G Stone, K Wang, V Gopalan, N Alem
Microscopy and Microanalysis 22 (S3), 914-915, 2016
28. **Aberration Corrected Scanning Transmission Electron Microscopy of (Ca, Sr)Fe₂O₅ Brownmillerite superlattices**
D Mukherjee, G Stone, EJ Moon, J Young, V Gopalan, J Rondinelli, S May, ...
APS March Meeting Abstracts 2016, X30. 012, 2016

Preprint

1. **Quantifying the coupling between strain and cation valence in high entropy oxide thin films using electron microscopy**
S Venkata Gayathri Ayyagari, SSI Almishal, D Mukherjee, ...
arXiv e-prints, arXiv: 2605.21612, 2026

2. **CryoBlob–A Feature Detection Tool for Low Dose CryoEM**
D Mukherjee, SR Brown, AL Jones, CAL Brantley, M Toro-Gonzalez, ...
Available at SSRN 6905758, 2026
3. **Predicting High-Resolution Spatial and Spectral Features in Mass Spectrometry Imaging with Machine Learning and Multimodal Data Fusion**
DM Mohammad Inzamam Ul Haque, Ramakrishnan Kannan, Jacob Daniel Hinkle ...
bioRxiv, 2025.02. 19.639070, 2025
4. **VISION: Toward a Standardized Process for Radiology Image Management at the National Level**
K Knight, I Danciu, O Ovchinnikova, J Hinkle, MC Shekar, D Mukherjee, ...
arXiv preprint arXiv:2404.18842, 2024
5. **Interlaced scan patterns based on progressive hexagonal grids**
JD Hinkle, D Mukherjee
arXiv preprint arXiv:2212.03356, 2022

Granted patent

1. **Machine learning on multimodal chemical and whole slide imaging data for predicting cancer labels directly from tissue images**
O S Ovchinnikova, J D Hinkle, I Haque, D Mukherjee
U.S. Patent US 12,675,875 B2; granted July 7, 2026

Commentary

1. **Operando imaging reveals nanocatalyst reconstruction: CO2 reduction**
D Mukherjee
Nature Catalysis 8 (6), 518-520, 2025

Software

1. **Janssen**
D Mukherjee, MJ Blake, BL Doughty, A Bryantseva
Undated record
2. **cryoblob**
D Mukherjee, AN Williams, S Cox, MT McDonell, A Borisevich
Undated record
3. **ptyrodactyl**
D Mukherjee, M Blake, B Doughty, S Retterer, R Sankaran
US Department of Energy (DOE) Software, 339, 2024
4. **DistGANS-Distributed Generative Adversarial Neural Networks**
M Lupo Pasini, V Gabbi, N Laanait, D Mukherjee, V Starchenko, J Yin, ...
US Department of Energy (DOE) Software, 13, 2022

Conference proceedings

1. **Cyber framework for steering and measurements collection over instrument-computing ecosystems**
A Al-Najjar, NSV Rao, R Sankaran, H Zandi, D Mukherjee, M Ziatdinov, ...
2023 IEEE International Conference on Smart Computing (SMARTCOMP), 198-200, 2023
2. **Image gradient decomposition for parallel and memory-efficient ptychographic reconstruction**
X Wang, A Tsaris, D Mukherjee, M Wahib, P Chen, M Oxley, ...
SC22: International Conference for High Performance Computing, Networking ..., 2022
3. **Enabling autonomous electron microscopy for networked computation and steering**
A Al-Najjar, NSV Rao, R Sankaran, M Ziatdinov, D Mukherjee, ...
2022 IEEE 18th International Conference on e-Science (e-Science), 267-277, 2022
4. **Virtual infrastructure twins: Software testing platforms for computing-instrument ecosystems**
NSV Rao, A Al-Najjar, H Zandi, R Sankaran, S Hicks, K Roccapriori, ...
Smoky Mountains Computational Sciences and Engineering Conference, 155-172, 2022

5. 26.5 Terahertz electrically triggered RF switch on epitaxial VO₂-on-Sapphire (VOS) wafer
H Madan, HT Zhang, M Jerry, D Mukherjee, N Alem, R Engel-Herbert, ...
2015 IEEE International Electron Devices Meeting (IEDM), 9.3. 1-9.3. 4, 2015

Thesis

1. Metrology of Ferroelectric Domain Walls with Scanning Transmission Electron Microscopy
D Mukherjee
The Pennsylvania State University, 2018
2. Structured semiconductor fibers for mid-infrared transmission
D Mukherjee
Boston University, 2013