

Debangshu Mukherjee

Materials science | Machine learning | Automated experiments

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Summary

Materials scientist combining hands-on electron microscopy, optical microscopy, and RHEED measurements with differentiable physics and GPU computing. Builds physical simulators and agent interfaces for scientific simulation and reconstruction.

Experience

Staff Scientist (R&D Associate), Oak Ridge National Laboratory

June 2021 – September 2026

- Connected electron microscopy with computing; coauthored work on networked instrument control, data transfer, and machine learning for experimental workflows.
- Coauthored SC22 ptychography study: a PbTiO₃ dataset with 16,632 probe positions reconstructed in 2.2 minutes on 4,158 GPUs (team result).

Postdoctoral Research Associate, Oak Ridge National Laboratory

June 2018 – April 2021

- First author of a 4D-STEM study measuring core-shell catalyst lattice strain with sub-picometer precision; developed robust atomic-position fitting methods.

Selected scientific software

Integrated chatbots with RHEED and ARPES simulators through automatons: discoverable AOT-compiled JAX workflows enable real-time simulation and reconstruction from a computer or phone during experiments.

- Janssen: differentiable wave optics and ptychographic phase retrieval. [GitHub](#) | [Docs](#)
- Ptyrodactyl: electron-scattering models and reconstruction. [GitHub](#) | [Docs](#)
- Rheedium: RHEED simulation and parameter fitting. [GitHub](#) | [Docs](#)
- diffpes: differentiable electronic-structure-to-ARPES simulation. [GitHub](#) | [Docs](#)

[CryoBlob](#) (cryo-EM features) · [Docs](#) | [stemtool](#) (STEM analysis) · [Docs](#)

Computational & experimental skills

Computing: JAX, PyTorch, automatic differentiation, inverse problems, Python, MATLAB, Dask, CuPy, GPU computing, and distributed analysis.

Experiments: Hands-on optical and electron microscopy, RHEED measurements; 4D-STEM, ptychography, strain mapping; angle-resolved photoemission spectroscopy (ARPES); focused ion beam preparation; chemical vapor deposition of 2D materials.

Education

Ph.D., Materials Science & Engineering — The Pennsylvania State University, 2018

M.S., Materials Science & Engineering — Boston University, 2013

B.Tech. (Honors) & M.Tech. — Indian Institute of Technology Kharagpur, 2011

Selected publications & patent

ML for automated STEM experiments — npj Computational Materials (2023), coauthor.

Image gradient decomposition for ptychography — SC22 (2022), coauthor.

4D-STEM lattice strain in core-shell electrocatalysts — ACS Catalysis (2020), first author.

US 12,675,875 B2 — granted July 7, 2026

Co-inventor: multimodal chemical and whole-slide imaging for cancer prediction.

Awards & honors

MAS Postdoctoral Scholar Award (2020) · Dean's Fellowship, Boston University (2011) · Best Bachelor's Thesis Award, IIT Kharagpur (2010).