Stanford



Ruchika Mahajan

Postdoctoral Scholar, Photon Science, SLAC

Bio

BIO

Ruchika Mahajan is a Postdoctoral Research Fellow at the SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University and SLAC National Accelerator Laboratory. Her research combines first-principles simulations, microkinetic modeling, and machine learning to understand and design functional materials, from strongly correlated transition-metal oxides to electrocatalysts for CO2 reduction.

She received her Ph.D. and M.Sc. (Integrated Ph.D.) from the Indian Institute of Technology (IIT) Mandi, India, in 2022, where she studied MnO2 polymorphs using Hubbard-corrected density functional theory (DFT+U, DFT+U+V) and computed magnetic exchange interactions with automated AiiDA workflows. Her work on intersite Hubbard interactions has been published in Physical Review Materials the Journal of Physical Chemistry C, and Physical Review B.

At SUNCAT, she develops open-source software and AI-ready data infrastructure for computational and experimental catalysis. She is the lead developer of the Experimental Catalysis Hub (CatHub), AutoCatLab (high-throughput DFT and COHP bonding analysis), and AutoCatKinetics (automated microkinetic modeling), and she builds agentic LLM tools that run computational catalysis workflows. She also combines COHP-derived electronic descriptors with graph neural networks to predict catalyst stability and activity.

HONORS AND AWARDS

- State Merit Award (Mukhya Mantri Protsahan Yojana) Cash incentive of INR 75,000 awarded, Government of Himachal Pradesh, India (August 2015)
- Selected Participant, Yambo School on Electronic Excitations in Novel Materials (fully funded), International Centre for Theoretical Physics (ICTP), Trieste, Italy (January 2020)
- Student ModCon Program Participant (competitively selected, fully funded, Trillion Parameter Consortium (TPC26 Conference and Hackathon), Baltimore, MD, USA (May 2026)

PROFESSIONAL EDUCATION

- Doctor of Philosophy (Ph.D.), Indian Institute of Technology (IIT) Mandi, India , Physics (2022)
- Master of Science (M.Sc.), Indian Institute of Technology (IIT) Mandi, India , Physics (2017)
- Bachelor of Science (B.Sc.), Govt. College Dharamshala, Himachal Pradesh University, India , Physics Hon's (2015)

STANFORD ADVISORS

- Thomas Jaramillo, Postdoctoral Faculty Sponsor

LINKS

- Experimental Catalysis Hub: https://experimental.catalysis-hub.org/
- AutoCatLab: https://github.com/SUNCAT-Center/AutoCatLab
- GitHub: https://github.com/ruchikamahajan66

- Linkedin: https://www.linkedin.com/in/ruchika-mahajan-9137ba126/
- Google Scholar: https://scholar.google.com/citations?user=amiJd_QAAAAJ&hl=en

Publications

PUBLICATIONS

- **Data as the Backbone of Artificial Intelligence: Insights from Heterogeneous Catalysis** *ACS CATALYSIS*
  Shin, D., Mahajan, R., Lian, Z., Heinlein, J., Cargnello, M., Tassone, C. J., Winther, K. T.
  2026
- **Comparative study of magnetic exchange parameters and magnon dispersions in NiO and MnO from first principles** *PHYSICAL REVIEW B*
  Dos Santos, F., Binci, L., Menichetti, G., Mahajan, R., Marzari, N., Timrov, I.
  2026; 113 (2)
- **A research database for experimental electrocatalysis: Advancing data sharing and reusability.** *The Journal of chemical physics*
  Mahajan, R., Aleman, A. M., Crago, C. F., Bhasker-Ranganath, S., Kreider, M. E., Zamora Zeledon, J. A., Schröder, J., Kamat, G. A., Hubert, M. A., Nielander, A. C., Jaramillo, T. F., Stevens, M. B., Voss, et al
  2025; 163 (12)
- **Pivotal Role of Intersite Hubbard Interactions in Fe-Doped α-MnO₂** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Mahajan, R., Kashyap, A., Timrov, I.
  2022; 126 (30): 14353-14365
- **Importance of intersite Hubbard interactions in β-MnO₂: A first-principles DFT plus U plus V study** *PHYSICAL REVIEW MATERIALS*
  Mahajan, R., Timrov, I., Marzari, N., Kashyap, A.
  2021; 5 (10)

PRESENTATIONS

- AutoCatLab: An Automated High-Throughput Framework for Generating Electronic Descriptors for Catalysis - Materials Research Society (MRS) Spring Meeting 2026
- Automated COHP Calculations for the Prediction of Stability and Catalytic Activity in Mixed Transition Metal Oxides - 29th North American Catalysis Society Meeting (NAM29)
- Pivotal Role of Intersite Hubbard Interactions in MnO2 Polymorphs - 33rd IUPAP Conference on Computational Physics (CCP2022)
- Importance of Intersite Hubbard Interactions in β-MnO2: A First-Principles DFT+U+V Study - ICTP Condensed Matter and Statistical Physics (CMSP) Section, Atomistic Simulation Webinar Series