

Toulik Maitra

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EDUCATION

University of California, Davis *GPA: 4.0*

Davis, CA

Doctor of Philosophy, Chemical Engineering

Sep. 2022 – 2027

- Awards: Recipient of UCD Graduate Research Award Fellowship (2025); Second Place in CHMS Symposium Outstanding Poster 2023; Top 60 in North America for Neutron and X-ray Scattering School (ANL/ORNL).

University of Calcutta *GPA: 8.36/10.0*

Kolkata, India

Bachelor of Technology, Chemical Engineering

Aug. 2016 – Aug 2020

- Awards: Best Paper Award at IIT Kharagpur; Most Innovative Idea in Nanoscience at IIT Bombay; Top 10 Team (out of 2500) in Global Entrepreneurship Event at IIT Kharagpur.

PROFESSIONAL EXPERIENCE

Graduate Student Researcher

Jan 2023 – Present

University of California, Davis

Davis, USA

- Developed a novel quantification method for structural disorder in organic semiconducting (OSC) materials, integrating experimental data (INS, XRD) with computational simulations.
- Designed quantitative and ML models based on phonon scattering data, contributing to improved material property validation.
- Implemented Monte Carlo and Molecular Dynamics methods to generate and validate diverse crystal structures; reparameterized force fields using DFT and DDEC6 computations.
- Co-authored a publication in a leading journal, demonstrating advanced modeling and simulation capabilities in material science.

Teaching Assistant

Apr 2023 – Present

University of California, Davis

Davis, USA

- Instructed seven diverse chemical engineering courses, emphasizing thermodynamics and unit operations fundamentals.
- Collaborated with faculty to enhance curriculum development and assess student performance.

Business Development Intern

May 2019 – Jul 2019

TATA Autocomps Systems Ltd

Pune, India

- Developed strategic cost-effectiveness assessments for internal production facilities (Top 5 projects).
- Synthesized comprehensive reports for senior management, informing process improvements.

Undergraduate Research Assistant

Feb 2018 – Dec 2021

University of Calcutta

Kolkata, India

- Investigated mass transfer and reaction kinetics in spinning basket membranes for protein recovery, correlating simulation results with experimental findings [Rana et al., 2021].
- Engineered hierarchical nanostructures for photovoltaics and water-splitting applications using DFT simulation techniques, referencing [Maitra et al., Energy & Fuels, 2021].
- Co-authored six peer-reviewed research publications, focusing on advanced material characterization and novel process design.
- Established and led university-level entrepreneurship clubs to foster innovation and cross-functional collaboration.

LEADERSHIP EXPERIENCE

E-Search Mentor, Summer 2024

- Guided an undergraduate in Mechanical and Aerospace Engineering at UC Davis on novel quantification methods for molecular disorder in OSCs.
- Supported the presentation of research findings at the UC Davis College of Engineering.

Co-Founder, eCell University of Calcutta

- Built and led a founding team to organize seminars/workshops aimed at enhancing entrepreneurship and innovation.
- Conducted over 50 interviews to identify new business ideas and foster student-led initiatives.

SELECTED PUBLICATIONS

- F. Maleki, **T. Maitra**, C.-W. Chiang, M. Dettmann, L.L. Daemen, J.E. Anthony, A.J. Moulé. *Extensive model validation enables quantitative prediction of complex structural and electronic properties*. (Under review)
- F. Maleki, K.J. Thorley, H.F. Iqbal, D. Vong, **T. Maitra**, L.L. Daemen, O.D. Jurchescu, J.E. Anthony, A.J. Moulé. *Design Rules to Optimize Intermolecular and Long-Range Packing of Organic Semiconductor Crystals*. **Chem. Mater.** 36(9), 4794–4805, 2024.
- K. Rana, **T. Maitra**, I. Saha, A. Saha, S. Gupta, D. Sarkar. *Modeling, simulation, and characterization of spinning basket membrane module in recovery of proteins from synthetic wastewater*. **J. Water Process Eng.** 42:102135, 2021.
- S. Maitra, S. Pal, **T. Maitra**, S. Halder, S. Roy. *Solvothermal etching-assisted phase and morphology tailoring in highly porous CuFe₂O₄ nanoflake photocathodes for solar water splitting*. **Energy & Fuels** 35(17), 14087–14100, 2021.
- S. Maitra, S. Halder, **T. Maitra**, S. Roy. *Superior light absorbing CdS/vanadium sulphide nanowalls@TiO₂ nanorod ternary heterojunction photoanodes for solar water splitting*. **New J. Chem.** 45, 7353–7367, 2021.
- S. Maitra, S. Pal, S. Datta, **T. Maitra**, B. Dutta, S. Roy. *Nickel doped molybdenum oxide thin film counter electrodes as a low-cost replacement for platinum in dye-sensitized solar cells*. **Mater. Today: Proc.** 39, 1856–1861, 2021.
- S. Maitra, A. Sarkar, **T. Maitra**, S. Halder, K. Kargupta, S. Roy. *Solvothermal phase change induced morphology transformation in CdS/CoFe₂O₄@Fe₂O₃ hierarchical nanosphere arrays as ternary heterojunction photoanodes for solar water splitting*. **New J. Chem.** 45, 12721–12737, 2021.
- S. Maitra, A. Sarkar, **T. Maitra**, S. Halder, S. Roy, K. Kargupta. *Cadmium sulphide sensitized crystal facet tailored nanostructured nickel ferrite @ hematite core-shell ternary heterojunction photoanode for photoelectrochemical water splitting*. **MRS Adv.** 5(50), 2585–2593, 2020.

SKILLS AND ACTIVITIES

Technical Languages: Python, C/C++, Bash, Linux, SQL (Postgres), R, MATLAB, PyTorch

Experimental Tools: Inelastic Neutron Scattering (INS), XRD, SEM, TEM, SAXS and GIWAXS

Personal Interests: Active athlete: Soccer and long-distance running; Reading interests: Historical fiction and fantasy genres