Toulik Maitra

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EDUCATION

University of California, Davis   *GPA: 4.0/4.0*   Davis, CA
Doctor of Philosophy, Chemical Engineering   *Sep. 2022 – 2026*

- <u>Awards</u>: Secured an External Fellowship from UCD Graduate Studies, 2025; Awarded the UCD Graduate Research Award Fellowship, 2025; Second Place in CHMS Symposium Outstanding Poster 2023; One of the top 60 graduate students in North America for Neutron and X-ray Scattering School (ANL/ORNL).
- <u>Relevant Courses</u>: Condensed Matter Physics, Theoretical Computational Chemistry, Quantum Chemistry (A and B), Advanced Functional Materials.

University of Calcutta   *GPA: 8.36/10.0*   Kolkata, India
Bachelor of Technology, Chemical Engineering   *Aug. 2016 – Aug 2020*

- <u>Awards</u>: 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

Visiting Fellow at Molecular Electronics Group   July 2025 – Present
Max Planck Institute for Polymer Research   *Mainz, Germany*

- Developed Polarizable Force Fields for thermally activated delayed fluorescence (TADF) emitters.
- Contributed to VOTCA software package integrating Jensen Model energy calculations for OLED materials.
- Developed a density of states (DOS) calculation methodology for TADF materials.

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

- **T. Maitra**, Chih-Hsuan Yang, Chen-Wei Chiang, Rachel L. Long, Cole David Brown, Baskar Ganapathysubramanian, A.J. Moulé. *A Voxelization Approach for Correlating MD with INS to Study Local and Global Structural Disorder.* (Under review)

- 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 $CuFe_2O_4$ 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