Toulik Maitra

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Education

University of California, Davis ***GPA: 4.0/4.0*** Davis, CA

PhD, Chemical Engineering (Advisor: Adam Moule) *Sep 2022 – Present*

- Research in semiconductor materials and interfaces connecting material disorder, stability, and performance through computation and experiment.
- Awards: Graduate Research Award Fellowship (2025); UCD Graduate Studies Fellowship (2025); CHMS Symposium Outstanding Poster (2023).

University of Calcutta ***GPA: 8.36/10.0*** Kolkata, India

BTech, Chemical Engineering *Aug 2016 – Aug 2020*

- Undergraduate research in nanomaterials and interfaces with results published in peer reviewed journals.
- Awards: Best Paper (IIT Kharagpur), Most Innovative Idea in Nanoscience (IIT Bombay), Among top 10 teams at Global Entrepreneurship Event (IIT Kharagpur).

Technical Skills

- **Experimental:** Semiconductor and materials modeling, process simulation, electronic structure analysis, data validation, device optimization
- **Characterization:** XRD, SEM, INS, TEM, PLS, XPS, EDAX, DSC, UV/VIS analysis; Spin-Coating and Solvothermal synthesis
- **Computational:** Python, MATLAB, C/C++, data analysis with Pandas/NumPy, finite element simulation (COMSOL, ANSYS)
- **Quantitative Methods:** Time series analysis, stochastic processes, regression, Monte Carlo simulation, optimization
- **Modeling & Analysis:** Statistical inference, data visualization, feature engineering, risk modeling, model validation
- **Essential Skills:** Technical writing, presentation skills, fast learner, team player, organization and management skills

Experience

Visiting Fellow, Molecular Electronics Group Jul 2025 – Present

Max Planck Institute for Polymer Research (Advisors: Denis Andrienko, Paul W.M. Blom) *Mainz, Germany*

- Developed polarizable force fields and simulation workflows for OLED (TADF) devices, boosting materials screening throughput by 30%.
- Collaborated with experimentalists to link polymer/crystal morphology to device architecture, achieving a 20% improvement in optical/electronic efficiency.
- Enhanced optical/electronic property prediction in VOTCA, improving FF parameterization accuracy by 60%.

Graduate Student Researcher Jan 2023 – Present

University of California, Davis *Davis,CA*

- Led computational analysis projects integrating DFT and multiphysics modeling with experimental data for process reliability.
- Created data pipelines to translate physical metrics into actionable performance indicators, improving decision efficiency by 35%.
- Collaborated with interdisciplinary teams to evaluate risks and optimize material use in high value components.

Teaching Assistant (TA) Apr 2023 – Mar 2025
University of California, Davis *Davis, USA*

- Taught 7 courses with class sizes averaging 150+ students each (1,000+ total), developed coursework in thermodynamics, materials processing, and transport phenomena, and collaborated with faculty to improve content delivery.

Business Development Intern May 2019 – Jul 2019
TATA Autocomp Systems Ltd *Pune, India*

- Collaborated with mechanical engineers on cost–performance tradeoffs for automotive components, reducing costs by $100K.
- Exposure to industrial-scale manufacturing and process optimization informed later focus on process–structure–performance modeling.

Summer Intern May 2018 – Jul 2018
Jadavpur University *Kolkata, India*

- Ran CFD simulations with probabilistic parameter sweeps; reduced computational cost by 20% through optimized algorithms.
- Quantified sensitivity of droplet–flame interactions, producing models transferable to risk and reliability analysis.

Winter Intern Feb 2018
Aditya Birla Group *Renukoot, India*

- Performed statistical process control analysis, identifying 15% reduction in bottlenecks in scaling operations.

Undergraduate Research Assistant Feb 2018 – Dec 2021
University of Calcutta *Kolkata, India*

- Modeled optical absorption/charge transport in hybrid nanostructures; demonstrated transferable methods for correlating structure, process, and performance.
- Studied thin-film structure–property correlations with relevance to energy and display devices, providing transferable insight to metallurgy process modeling.

Leadership and Initiatives

Served as a peer reviewer for ACS Omega, evaluating manuscripts in the field of nanomaterials and physical chemistry.

Supervised a team of undergraduates in developing machine learning workflows for material performance prediction.

Co-founded the Entrepreneurship Cell at University of Calcutta; organized prototyping workshops and mentoring sessions.

Publications (7 out of 10)

- Felix Post,Jean-Philip Filling, **T. Maitra**, Michael Wand, Denis Andrienko. *Parametrization of distributed polarizable force fields.* (Under review)
- **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 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.