

Toulik Maitra

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EDUCATION

University of California, Davis	GPA: 4.0/4.0	Davis, CA
<i>PhD, Chemical Engineering (Advisor: Adam Moule)</i>		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
<i>BTech, Chemical Engineering</i>		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
<i>Max Planck Institute for Polymer Research (Advisors: Denis Andrienko, Paul W.M. Blom)</i>	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
<i>University of California, Davis</i>	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
<i>University of California, Davis</i>	<i>Davis, USA</i>
– 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
<i>TATA Autocomp Systems Ltd</i>	<i>Pune, India</i>
– 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
<i>Jadavpur University</i>	<i>Kolkata, India</i>
– 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
<i>Aditya Birla Group</i>	<i>Renukoot, India</i>
– Performed statistical process control analysis, identifying 15% reduction in bottlenecks in scaling operations.	
Undergraduate Research Assistant	Feb 2018 – Dec 2021
<i>University of Calcutta</i>	<i>Kolkata, India</i>
– 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.	
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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.	
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PUBLICATIONS	
<ul style="list-style-type: none"> • Félix Post, Jean-Philip Filling, T. Maitra, Michael Wand, Denis Andrienko. <i>Parametrization of distributed polarizable force fields.</i> (Under review) • T. Maitra, Chih-Hsuan Yang, Chen-Wei Chiang, Rachel L. Long, Cole David Brown, Baskar Ganapathysubramanian, A.J. Moulé. <i>A Voxelization Approach for Correlating MD with INS to Study Local and Global Structural Disorder.</i> (Under review) • F. Maleki, T. Maitra, C.-W. Chiang, M. Dettmann, L.L. Daemen, J.E. Anthony, A.J. Moulé. <i>Extensive model validation enables quantitative prediction of complex structural and electronic properties.</i> (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. <i>Design Rules to Optimize Intermolecular and Long-Range Packing of Organic Semiconductor Crystals.</i> Chem. Mater. 36(9), 4794–4805, 2024. • K. Rana, T. Maitra, I. Saha, A. Saha, S. Gupta, D. Sarkar. <i>Modeling, simulation, and characterization of spinning basket membrane module in recovery of proteins from synthetic wastewater.</i> J. Water Process Eng. 42:102135, 2021. • S. Maitra, S. Pal, T. Maitra, S. Halder, S. Roy. <i>Solvothermal etching-assisted phase and morphology tailoring in highly porous CuFe₂O₄ nanoflake photocathodes for solar water splitting.</i> Energy & Fuels 35(17), 14087–14100, 2021. • S. Maitra, S. Halder, T. Maitra, S. Roy. <i>Superior light absorbing CdS/vanadium sulphide nanowalls@TiO₂ nanorod ternary heterojunction photoanodes for solar water splitting.</i> 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.