Asmita Jana, Ph.D.

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Profile:

Computational Materials Scientist with **8+ years** of experience with **Density Functional Theory, Molecular Dynamics, and Machine Learning** for molecular and materials design in energy technology applications. Experience includes **electrochemical interfaces, reaction kinetics, complex process engineering experiments, surface interactions, free energy calculations, mechanical properties, characterization, thermal effects, transport phenomena, and data analysis**. Published in top journals, thrives in collaborative teams, and has excellent programming skills.

Education:

Massachusetts Institute of Technology — Cambridge, US
Ph.D. in Materials Science and Engineering — Sep. 2017- Aug. 2022

Indian Institute of Technology Madras — Chennai, India
B.Tech. and M. Tech. in Metallurgical and Materials Engineering — Aug. 2012- Jul. 2017

Key accomplishments:

- Authored **16** peer-reviewed publications in journals like Nature Catalysis, Nature Computational Science, and Science Advances; Research highlighted by **MIT News, Elements, and ALS News**
- Delivered **10+** talks/posters on research findings including 2 invited talks at UC symposiums
- **Editorial Board member** of Discover Catalysis and Discover Surfaces journals

Research Experience:

Lawrence Berkeley National Laboratory — Berkeley, CA
Postdoctoral Researcher | Chemical Sciences Division — Sep. 2022- Present

- Worked on **10+ modeling projects** and collaborated with **15+ multidisciplinary collaborators** in modeling complex electrochemical interfaces, catalytic reactions, adsorption, and solvation using DFT, MD, and ML
- Built and validated **predictive modeling workflows** by **benchmarking ML interatomic potential** models (UMA, eSEN) and datasets (OC20, OC25, OMat24) against **DFT** for water splitting reaction
- Trained **graph neural networks (CGCNN)** for property prediction (dielectric constant, band gap) using Matminer datasets; implemented preprocessing, training, validation, & testing pipelines in Python
- Designed **descriptor-based modeling** approaches linking structure/chemistry of **electrocatalysts** to performance-relevant trends (stability of intermediates, interfacial microenvironment formation)
- Enhanced **reaction rate** of CO_2RR over HER by stabilizing *COOH **>2 fold** through mechanistic modeling of microenvironment, converted mechanistic insight into actionable optimization levers
- Developed an **ML-based Digital Twin** that connects **multimodal characterization (XPS, FTIR)** to chemical insights; demonstrated **rapid kinetic inference** using **6 XPS spectra in <10 minutes**, enabling a practical model-experiment feedback loop
- Devised and evaluated criteria for graphene-based functionalizations as optimal CO_2 solid adsorbents including optimal adsorption energy, thermal stability, defect insensitivity, selectivity, and capacity

Massachusetts Institute of Technology — Cambridge, MA
Graduate Researcher | Dept. of Materials Science and Engineering — Oct. 2017- Aug. 2022

- Modeled coupled **chemistry–transport–structure** problems across membranes, surfaces, and manufacturing processes, collaborating with **10+ scientists** across academia, national labs, and industry.

- Created a **reactive MD workflow** to simulate **processing → chemistry → structure → mechanical properties** in pitch-based carbon fiber formation by explicitly modeling crosslinking reactions; identified a pathway toward **lower-cost manufacturing**.
- Developed a combined **classical MD + DFT** workflow demonstrating **>5× selectivity** (O_2 vs N_2) through a 2D nanoporous membrane template, showing skill in turning complex simulations into performance-driving descriptors.
- Demonstrated **>2× change in water permeation rate** in functionalized graphene by isolating chemical effects (hydrophobic vs hydrophilic), highlighting strength in connecting surface chemistry to transport and performance.

Domain Knowledge:

- Fields: Interfacial interactions, Reaction kinetics, Electrochemistry, Adsorption, Characterization, Ion transport, Mechanical properties
- Materials: Metals, Metal oxides, Organic molecules, Water, Gas, Graphene, Graphene Oxide, Nano-porous materials, Aerosols, Carbon Fibers
- Systems: Catalysts, Membranes, Adsorbents

Skills:

- Quantum Mechanics: VASP, ORCA, Quantum ESPRESSO, TeraChem, CP2K
- Molecular Dynamics: LAMMPS; Classical FFs (OPLS), ReaxFF, and MLIPs
- Machine Learning: PyTorch, Tensorflow, Keras, Scikit-learn
- Machine Learning models: CGCNN (graph NN), MACE, UMA, eSEN
- Machine Learning datasets: OC20, OC25, OMat24, OMol25, Matminer
- Programming languages: Python, C, C++, Fortran, Matlab, Bash
- Python libraries: NumPy, PyTorch, ASE, Pandas, Matplotlib, RDKit
- Systems: HPC, Slurm, MPI, OpenMP, GPUs, Git, Linux
- Thermodynamic modeling: Thermo-Calc, FactSage, Calphad method

Leadership, Communication, and Outreach:

- MIT Teaching Leadership: led instruction with **20+ TAs for 500+ students** in Solid State Chemistry, MIT (2019)
- Mentorship: supervised/mentored **~5** graduate/undergraduate researchers and interns
- Cross-functional leadership: led research updates across **15+ multidisciplinary teams**
- Public speaking: **LBNL Slam finalist (2023)**; lightning round winner (Gerischer electrochemistry conference)
- Symposium leadership: chaired ACS Fall 2023 electrocatalysis session (~15 presenters)
- Volunteering: **10+** activities; communicated my research in local community including elementary, middle, and high school students, undergraduates in ACS, and underrepresented communities

Selected Publications (Total 16):

Shan, Y., Zhao, X., Fonseca, G. M., **Jana, A.**, *et al.* "Nanometre-resolved observation of electrochemical microenvironment formation at the nanoparticle-ligand interface." **Nature Catalysis** (2024): 1-10. ***Highlighted in LBNL newsletter- Elements and ALSNews***

Jana, A., *et al.* "Atoms to Fibers: identifying novel processing methods in the synthesis of pitch-based carbon fibers." **Science Advances** (2022): 8(11), eabn1905. ***Highlighted in MIT News and other media outlets***

Jana, A., *et al.* "Benchmarking Machine-Learned Potentials for Water-Splitting Catalysts: Validation on Pt and IrO_2 Surfaces Using OC20 and OMat24", ChemRxiv, 29 January 2026, DOI: https://doi.org/10.26434/chemrxiv.10001728/v1

Jana, A., *et al.* "Mechanistic study of CO_2 reduction in a metal/nanoparticle/ligand-based nanoconfined pocket" (in preparation)