Asmita Jana, Ph.D.

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Profile:

Computational Materials Engineer with 8+ years of experience with **Density Functional Theory, Molecular Dynamics simulations, and Machine Learning** for molecular and materials design in energy technology applications. Experience includes simulating **complex process engineering experiments, surface interactions, reaction kinetics, characterization, thermal effects, transport phenomena, electrochemical performance, 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 **15** 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

Research Experience:

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

- Worked on **10+** projects and collaborated with **15+** multidisciplinary scientists in modeling complex electrochemical interfaces, catalytic reactions, adsorption, and solvation using DFT, MD, and ML
- Using **ML model** (UMA, Meta) to create modeling workflow for predicting catalytic properties for water splitting reaction and CO_2 reduction reaction
- Trained **CGCNN** to predict dielectric constant & band gap from data sets in **Matminer database**
- Designed **ML-based Digital Twin** to simulate characterization tools like XPS and FTIR and used ML to predict **surface reaction kinetics** with just **6 XPS spectra in <10 mins**
- Created better **hybrid metal nanoparticle/organic ligand** electrocatalysts by increasing the stability of the **nanoconfined interfaces** and CO_2RR intermediates by > **2-fold** to enhance reaction rate using **DFT**
- 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

- Worked on **5** projects and collaborated with **10+** multidisciplinary scientists from academia, national labs, and industries in modeling membrane permeation, adsorption on transition metal oxides, and the manufacturing process and mechanical properties of carbon fibers
- Created a reactive MD **workflow to simulate the carbon fibers manufacturing process** with accurate mechanical properties by simulating the crosslinking reactions of precursor organic molecules; discovered **new pathway** to make **cheaper carbon fibers**
- Obtained **>5-fold** permeability difference between O_2 and N_2 gas in 2D nanoporous membrane template by developing a workflow with classical MD and DFT

- Demonstrated **>2-fold** permeation rate of water in graphene with hydrophobic functionalization like epoxide compared to hydrophilic like hydroxyl using classical MD

Indian Institute of Technology Madras Chennai, India
Graduate Researcher | Dept. of Metallurgical and Materials Engineering Apr. 2016- Jul. 2017

- Added the Ni-Zr phase diagram to the **SGTE thermodynamic database (total 2773 datasets)** by creating it using Calphad method with experimental and DFT enthalpies of formation data as input

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
- Machine Learning datasets: OC20, OC22, 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
- Multiphysics modeling: ABAQUS

Leadership, Communication, and Outreach:

- Led classroom instruction with **20+** TAs for **500+** students in Solid State Chemistry, MIT (2019)
- Supervised and mentored ~**5** graduate and undergraduate students including interns
- Led research updates within **15+** multidisciplinary teams from academia, national labs, and industries
- Chaired electrocatalysis symposium with **~15** presenters at ACS Fall 2023
- Finalist in LBNL Slam 2023 and winner of lightning round at 2nd Gerischer electrochemistry conference, competitions for **public speaking** about my research
- Volunteered in **10+** activities; communicated my research in local community including elementary, middle, and high school students, undergraduates in ACS, and underrepresented communities

Selected Publications (Total 15):

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.* "Designing the nanoconfined environment for energy-efficient metal nanoparticle/ligand-based electrocatalysts." The Journal of Physical Chemistry Letters (2025): 16, 5769-5778

Qian, J., **Jana, A.**, *et al.* "DTCS for Chemical Science: a case study on water interactions on the Ag(111) surface". **Nature Computational Science** (2025): 1-8