Asmita Jana, Ph.D.

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Profile:

Computational Materials Engineer with 7+ years of experience with **Density Functional Theory, Molecular Dynamics simulations, and Machine Learning** for property prediction and structure-to-function modeling in catalysts and energy materials. Experience includes simulating **complex process engineering experiments, surface interactions, reaction kinetics, characterization, thermal effects, transport phenomena, electrochemical performance, and data analysis** in energy technology applications. 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

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 forcefields, ReaxFF, and MLIPs
- Programming languages: Python, C, C++, Fortran, Matlab, Bash
- Python libraries: NumPy, PyTorch, ASE, Pandas, Matplotlib, RDKit
- Systems: HPC, Slurm, MPI, OpenMP, GPUs, Git, Linux
- Machine Learning: PyTorch, Tensorflow, Keras, Scikit-learn
- Visualization: VMD, Avogadro, Ovito, VESTA
- Thermodynamic modeling: Thermo-Calc, FactSage, Calphad method
- Finite Element Analysis: ABAQUS

Key accomplishments:

- Authored **15** peer-reviewed publications in journals like Nature Catalysis, Nature Computational Science, Science Advances, and Small
- Research highlighted by **MIT News, Elements, ALS News**, and other media outlets

Research Experience:

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

- **Modeling interface of nanoconfined electrocatalysts:**
  - Investigated the structure-function relationship in **metal/ligand complexes** under electrochemical potentials and optimized the environment for better performance using DFT
  - Demonstrated **>2 fold** stability of CO_2 reduction reaction intermediates leading to enhanced reaction rate in nanoconfined interfaces

- Applying **ML model** (UMA, Meta) to create modeling workflow for predicting catalytic properties for water splitting reaction

- **Machine Learning to predict surface reaction kinetics:**
  - Part of a team that used global optimization and machine learning to predict reaction mechanisms and rates from XPS spectra
  - Generated highly accurate and non-degenerate solutions with **just 6 spectra in <10 mins**

- **Carbon capture using functionalized graphene:**
  - Quantified key energetic parameters like thermal stability to predict best CO_2 solid adsorbents
  - Evaluated them for functionalized, doped, and defective graphene using DFT

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

- **Modeling framework to generate carbon fibers:**
  - Simulated carbon fibers manufacturing process from heterogeneous organic molecules of varying shape, size, and functionalization using MD with ReaxFF to model reactions
  - Created descriptor to determine degree of crosslinking; simulated fibers match experimental mechanical properties like elastic modulus
  - Discovered **new pathway** to generate **cheaper carbon fibers** with improved tensile and compressive modulus

- **Water and Gas permeation through graphene-based membranes:**
  - Demonstrated **>2 fold** permeation rate of water in graphene with hydrophobic functionalization like epoxide compared to hydrophilic like hydroxyl using classical MD
  - Obtained **>5 fold** permeability difference between O_2 and N_2 gas a 2D nanoporous membrane template using a workflow with classical MD and DFT
  - Showed that membranes from Fe_2O_3 and Co_3O_4 can separate O_2 from air

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

- **Ni-Zr phase diagram:**
  - Added to the **SGTE thermodynamic database (total 2773 datasets)** by creating the Ni-Zr phase diagram using Calphad method with experimental and *ab initio* data as input
  - Calculated formation enthalpies of intermediate phases in the Ni-Zr and Al-Ni-Zr using DFT

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: A blueprint for digitizing chemistry characterizations". **Nature Computational Science** (2025) (Accepted)

Patil, J. J., Lu, Z., Zachman, M. J., Chen, N., Reeves, K. S., **Jana, A.**, *et al.* "Chemical and physical drivers for improvement in permeance and stability of linker-free graphene oxide membranes." Nano Letters (2023): 23(14), 6414-6423.