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 pathway analysis, ion transport, electrochemical performance, and data analysis using machine learning 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: Reaction kinetics, Interfacial interactions, electrochemistry, adsorption, characterization, mass transport, mechanical properties
- Materials: Organic molecules, Water, Gas, Graphene, Nanoporous materials
- 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
  - Using **ML** with UMA from Meta to obtain 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.

Jana, A., Bergsman, D. S., and Grossman, J. C. "Adsorption-based membranes for air separation using transition metal oxides." Nanoscale Advances (2021): 3(15), 4502-4512.