Asmita Jana, Ph.D.

Berkeley, CA | asmitajana@gmail.com | www.linkedin.com/in/asmitajana

Profile:

Computational Materials Engineer with 7+ years of experience with Density Functional Theory and Molecular Dynamics simulations 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
- Experienced with grant writing for DOE programs and mentoring and managing junior scientists
- Published in top journals, thrives in collaborative teams, and has excellent programming skills.

Domain Knowledge:

- **Fields:** Catalysis, Electrochemistry, Reaction Kinetics, Interfacial interactions, Thermodynamics, Adsorption, Materials and Surface Characterization, Mass transport, Mechanical properties
- **Materials:** Metal, Metal oxides, Organic ligands, Water, Gases: CO_2, O_2, N_2, H_2, Graphene, Graphene oxide, MOFs, Nano-porous materials, Carbon-based materials, Aerosols, and Carbon Fibers.
- **Systems:** Catalysts, Membranes, Adsorbents

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

Skills:

- **Quantum Mechanics:** VASP, Phonopy, ORCA, Quantum ESPRESSO, TeraChem, CP2K
- **Molecular Dynamics:** LAMMPS; Classical forcefields and ReaxFF, Machine Learning Interatomic Potentials (MLIPs)
- **Programming and software dev:** Python, C, C++, Fortran, Matlab, Linux (Bash, Vim), HPC (slurm, OpenMP, MPI, GPUs), ASE, NumPy, Pandas, Matplotlib
- **Machine Learning:** PyTorch, Tensorflow, Keras, Scikit-learn
- **Visualization:** VMD, Avogadro, Ovito, VESTA
- **Thermodynamic modeling and:** Thermo-Calc, FactSage, Calphad method
- **Finite Element Analysis:** ABAQUS
- **Graphic design and Typesetting:** Adobe Illustrator, LaTeX

Research Experience:

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

- **Modeling interface of nanoconfined electrocatalysts:** Used DFT to chart the evolution of metal/ligand electrocatalyst structure with applied potential until the nanoconfined interface is created. Developed descriptors to model stability of the nanoconfined interface as a function of ligand lengths, ligand densities, surface defects, and interfacial protons. Demonstrated that such interfaces accelerate the CO_2 reduction reaction by stabilizing the reaction intermediates.
- **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 X-ray Photoelectron Spectroscopy

spectra. Analyzed algorithms' performance by assigning scores and optimized for high accuracy and non-degeneracy.
- **Carbon capture using functionalized graphene:** Used DFT to calculate adsorption energy of CO_2 on functionalized, doped, and defective graphene to simulate activated carbon. Determined optimal range for adsorption energy in physisorption/chemisorption boundary. Calculated thermal stability, defect insensitivity, selectivity, and capacity for CO_2 adsorption for functionalizations in the optimal range.

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

- **Modeling framework to generate carbon fibers and evaluate mechanical properties:** Used MD with ReaxFF to simulate the generation of carbon fibers from crosslinking reactions in heterogeneous mixture of aromatic organic molecules of varying shape, size, and functionalization. Created descriptor to determine degree of crosslinking. Collaborated with experimental teams to ensure generation framework closely follows experimental procedure. Simulated carbon fibers match experimental mechanical properties like elastic modulus. Framework gave new insights into generating cheaper carbon fibers with improved compressive modulus.
- **Water permeation through graphene-based membranes:** Used Classical MD to simulate permeation of water through pristine and hydroxyl and epoxide functionalized graphene. Computed effect of pore size, pore functionalization, and graphene functionalization at various densities on water transport characteristics.
- **Air separation using adsorption-based membranes:** Performed classical MD to compute permeability and selectivity of oxygen and nitrogen gas through a 2D nanoporous membrane. By varying their adsorption energies, created a model to evaluate selectivity and permeability as a function of adsorption energy differences of gas species permeating through a pore-flow membrane. Used DFT to calculate adsorption energies of gases and determined some transition metal oxides that maximize performance.

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

- **Phase stability of Ni-Zr intermetallics to create Ni-Zr phase diagram:** Used DFT to calculate formation enthalpies of intermediate phases in the Ni-Zr and Al-Ni-Zr systems. Assessed the Ni-Zr phase diagram using the Calphad method with experimental and *ab initio* data as input.

Selected Publications:

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.

Jana, A., Sridar, S., Fries, S. G., Hammerschmidt, T., & Kumar, K. H. "Thermodynamic modelling of the Ni–Zr system." Intermetallics (2020), 116, 106640.