

# Asmita Jana

Computational Materials Scientist  
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## Research Interests

Computational Chemist with 8+ years of experience using **Density Functional Theory, Molecular Dynamics, and Machine Learning** for property prediction, materials discovery, and structure-to-function modeling 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**. Has written grant proposals, published in top journals, thrives in a collaborative team setting, and has excellent programming and communication skills.

## Education

### Massachusetts Institute of Technology

Ph.D. in Materials Science and Engineering  
GPA: 4.8/5

Advisor: Prof. Jeffrey C. Grossman

Thesis: Design of surface and bulk interactions: A computational approach to sustainable energy

Cambridge, USA

Sep 2017 – Aug 2022

### Indian Institute of Technology Madras

M.Tech. and B.Tech. in Metallurgical and Materials Engineering  
GPA: 9.63/10; Valedictorian

Advisor: Prof. K. C. Hari Kumar

Thesis: Thermodynamic optimization of the Ni-Zr system

Chennai, India

Aug 2012 – Jul 2017

## Skills

- **Quantum Mechanics:** VASP, Phonopy, ORCA, Quantum ESPRESSO, TeraChem, CP2K, ASE
- **Molecular Dynamics:** LAMMPS; Classical forcefields and ReaxFF, Machine Learning Interatomic Potentials (MLIPs)
- **Machine Learning:** PyTorch, Tensorflow, Keras, Scikit-learn
- **Machine Learning models:** UMA, MACE, CGCNN (graph NN), eSEN
- **Machine Learning datasets:** OC20, OC25, OMat24, OMol25, Matminer
- **Programming languages:** Python, C, C++, Fortran, MATLAB, Bash
- **Python libraries:** NumPy, PyTorch, ASE, Matplotlib, Pandas, RDKit
- **Systems:** HPC, Slurm, MPI, OpenMP, GPUs, Git, Linux
- **Visualization softwares:** VMD, Avogadro, Ovito, VESTA

- **Thermodynamic modeling:** Thermo-Calc, FactSage, Calphad method
- **Multiphysics modeling:** ABAQUS
- **Graphic design and Typesetting:** Adobe Illustrator, L<sup>A</sup>T<sub>E</sub>X

## 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<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, Graphene, Graphene oxide, MOFs, Nano-porous materials, Carbon-based materials, Aerosols, and Carbon Fibers
- **Systems:** Catalysts, Membranes, Adsorbents, Colloids

## Research Experience

**Chemical Sciences Division,  
Lawrence Berkeley National Laboratory**

Berkeley, USA

**Machine learning potentials for catalytic properties**

Jul. 2025 – Present

*Postdoctoral Researcher | Advisors: Dr. Jin Qian*

- 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
- Evaluating the long range interactions between ions and metal surfaces using pretrained MLIPs

**Chemical reaction energy landscape in nanoconfinement**

Feb. 2024 – Present

*Postdoctoral Researcher | Advisors: Dr. Ethan Crumlin, Dr. Jin Qian*

- Calculated the Gibbs free energies of the reaction intermediates in the CO<sub>2</sub> reduction to CO and hydrogen evolution reaction using DFT in nanoconfined interfaces with 2D confining surfaces and 3D organic ligand as confining species
- Enhanced the reaction rate of CO<sub>2</sub>RR over HER by stabilizing \*COOH >2 fold through mechanistic modeling of microenvironment; converted mechanistic insight into actionable optimization levers

**Digital Twin for digitizing chemical characterization**

Feb. 2024 – Present

*Postdoctoral Researcher | Advisors: Dr. Ethan Crumlin, Dr. Jin Qian*

- Part of a team that used global optimization and machine learning to predict reaction mechanisms and rates from X-ray Photoelectron Spectroscopy spectra; demonstrated rapid kinetic inference using 6 XPS spectra in <10 minutes, enabling practical model-experiment feedback loop

- Analyzed algorithms' performance by assigning scores and optimized for high accuracy and non-degeneracy
- Currently, extending the digital twin code to incorporate Infrared spectroscopy as a step towards simulating multimodal characterization

**Effect of pH on solvation in Ammonium sulfate aerosols** Nov. 2023 – May 2025  
*Postdoctoral Researcher* | Advisors: Dr. Musahid Ahmed, Dr. Jin Qian

- Simulated ammonium sulfate clusters under varying pH to observe solvation using DFT; quantified spatial distribution and coordination numbers
- Demonstrated that at higher pH, the water to sulfate ratio decreases
- Collaborated with an experimental team in LBNL

**Designing energy-efficient nanoconfined electrocatalysts** Sep. 2023 – Feb. 2025  
*Postdoctoral Researcher* | Advisors: Dr. Ethan Crumlin, Dr. Jin Qian

- Investigated the effect of ligand length, ligand density, surface defects, and presence of interfacial protons on nanoconfined pocket stability
- Simulated surface defects like Au and Cu dopants and Ag vacancies, in an Ag nanoparticle/ligand catalyst to decrease the potential needed for creating nanoconfinement
- Observed that increased ligand length, ligand density, Au dopants, and interfacial protons lower the transition potential

**Modeling nanoconfinement in an electrocatalyst** Nov. 2022 – Mar. 2023  
*Postdoctoral Researcher* | Advisors: Dr. Jin Qian

- Simulated an Ag nanoparticle/ligand-based electrocatalyst for carbon conversion using DFT and evaluated the structural features as a function of applied potential
- Developed a hypothesis to explain the phase space observed and validated the experimental observations
- Collaborated with two experimental teams from UC Berkeley

**Design rules for carbon capture using activated carbon** Sep. 2022 – Nov. 2023  
*Postdoctoral Researcher* | Advisor: Dr. Jin Qian

- Mentored a graduate student from University of Idaho performing DFT calculations and analyzed trends of carbon dioxide adsorption energy on functionalized graphene as a template material for activated carbon
- Created design rules based on electronegativity differences, defects on graphene, and thermal stability of the functional groups on graphene

**Department of Materials Science and Engineering,  
Massachusetts Institute of Technology** Cambridge, USA

**Water permeation through graphene-based membranes** Dec. 2021 – Aug. 2022  
*Graduate Researcher* | Advisors: Prof. Jeffrey Grossman, Dr. Nicola Ferralis

- Performed classical Molecular Dynamics (MD) simulations to simulate the permeation of water through pristine graphene layers as well as graphene layers functionalized with hydroxyl groups and epoxide groups
- Computed the effect of morphological changes of graphene layer on permeation characteristics
- Worked closely with experimental teams from Massachusetts Institute of Technology, National Energy Technology Laboratory, and Oak Ridge National Laboratory

### **Cross-linking reactions in methylated carbon fibers**

May. 2021 – Aug. 2022

*Graduate Researcher | Advisors: Prof. Jeffrey Grossman, Dr. Nicola Ferralis*

- Performed MD simulations with reactive forcefields on pyrene-based systems to simulate formation of carbon fibers and calculated the impact of methyl groups on elastic modulus
- Designed a parameter that can represent the number of cross-linked bonds formed during reactions
- Collaborated with experimental teams from Western Research Institute and Oak Ridge National Laboratory

### **New strategies to synthesize high modulus carbon fibers**

Oct. 2020 – Nov. 2021

*Graduate Researcher | Advisors: Prof. Jeffrey Grossman, Dr. Nicola Ferralis*

- Designed an experimentally validated framework to simulate the generation of coal-tar and petroleum pitch-based carbon fibers using MD simulations with reactive forcefields; calculated mechanical properties like elastic modulus
- Explored the parameter space and predicted new and cheaper synthesis strategies to generate high modulus carbon fibers
- Collaborated with multidisciplinary teams from Western Research Institute, Oak Ridge National Laboratory, and University of Wyoming

### **Adsorption-based membranes for air separation**

Nov. 2017 – Feb 2021

*Graduate Researcher | Advisor: Prof. Jeffrey Grossman*

- Created a model to evaluate the dependence of selectivity on adsorption energy differences of gas species permeating through a pore-flow membrane
- Performed classical MD simulations to calculate permeability and selectivity of oxygen and nitrogen gas through a 2D nanoporous membrane
- Used DFT to calculate adsorption energies of the gases at various configurations on some transition metal oxides

### **Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras**

Chennai, India

### **Thermodynamic Optimization of the Ni-Zr system**

May 2016 – May 2017

*Graduate Researcher | Advisor: Prof. K.C. Hari Kumar*

- Performed *ab initio* calculations and determined the enthalpies of formation of the intermediate phases in Ni-Zr and Al-Ni-Zr systems using DFT
- Assessed the Ni-Zr phase diagram using the Calphad method with experimental and *ab initio* data as input

**Interdisciplinary Centre for Advanced Materials Simulation,** Bochum, Germany  
**Ruhr Universität Bochum**

***Ab initio* calculations of the Ni-Zr system** May – Jul. 2016

*Intern* | Advisors: Dr. Suzana G. Fries and Dr. Thomas Hammerschmidt

- Used DFT to calculate enthalpies of formation of the intermediate phases and Phonopy to get heat capacities

**Centre for Research in Computational Thermochemistry,** Montréal, Canada  
**Polytechnique Montréal**

**Liquidus projections of molten salt systems** May – Aug 2015

*Intern* | Advisors: Prof. Patrice Chartrand and Dr. Christian Robelin

- Employed Modified Quasichemical model along with FactSage thermochemical software to optimize a binary system- BaCl<sub>2</sub>+BaF<sub>2</sub> and calculate the liquidus projection of four salt systems- Na, Ba//Cl, F; Sr, Ba//Cl, F; Li, Ba//Cl, F; K, Ba//Cl, F; and Ca, Ba//Cl, F

## Publications

- **Jana, A.**, Roncoroni, F., Fornaciari, J., Krishnapriyan, A. S., Prendergast, D., Weber, A., Crumlin, E. J., and Qian, J. “Benchmarking Machine-Learned Potentials for Water-Splitting Catalysts: Validation on Pt and IrO<sub>2</sub> Surfaces Using OC20 and OMat24.” ChemRxiv. 29 January 2026. DOI: <https://doi.org/10.26434/chemrxiv.10001728/v1>
- **Jana, A.**, Crumlin, E. J., and Qian, J. “Mechanistic study of CO<sub>2</sub> reduction in a metal/nanoparticle/ligand-based nanoconfined pocket” (in preparation)
- **Jana, A.**, Yang, P., Qian, J., and Crumlin, E. J. “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.**, Menon, S., Bogdan, A. E., Hamlyn R., Mahl, J., and Crumlin, E. J. “DTCS for Chemical Science: a case study on water interactions on the Ag(111) surface.” Nature Computational Science (2025): 1-8
- Greenspoon, E., Warkander, S., Kim, P., **Jana, A.**, Qian, J., Wilson, K. R., Ahmed, M., Bergner, J. “Soft X-ray spectroscopy of ammonium sulfate aerosols at varied pH conditions.” The Journal of Chemical Physics (2025): 162(23)
- Zhang, Z., Liu, L., Glenna, D. M., **Jana, A.**, Perez, C. M, and Qian, J. “Real-space Kohn-Sham density functional theory for complex energy applications.” Chemical Communications (2025)

- Meng, Y., Neupane, M., Glenna, D. M., **Jana, A.**, Wang, W., Zhao, H., Qian, J., Yang, Y., Wang, L., and Snyder, S. W. “Balsa Wood-derived carbon enriched with hydroxyl functional groups for efficient CO<sub>2</sub> sorption.” ACS Sustainable Chemistry and Engineering (2025): 13(16), 5974-5984
- Sambur, J. B., Kaufman, A. J., Montoya-Castillo, A., Kundman, A., Nozik, A. J., DesCarpentrie, A. G., **Jana, A.**, et. al. “Gerischer Electrochemistry Today.” ACS Energy Letters (2025): 10(12), 6578-6595
- Li, H.\* **Jana, A.\***, Garcia-Esparza, A. T., Li, X., Kaminsky, C., Hamlyn, R., Prabhakar, R., Atwater, H. A., Ager, J. W., Sokaras, D., Yano, J., and Crumlin, E. J. “When photoelectrons meet gas molecules: determining the role of inelastic scattering in Ambient Pressure.” ACS Central Science (2024): 11(1), 98-106. \* equal contribution.
- Shan, Y., Zhao, X., Fonseca, G. M., **Jana, A.**, Chen, S., Yu, S., Ng, K. C., Roh, I., Chen, H., Altoe, V., Corder, S. N. G., Bechtel, H. A., Qian, J., Salmeron, M., and Yang, P. “Nanometre-resolved observation of electrochemical microenvironment formation at the nanoparticle-ligand interface.” Nature Catalysis (2024): 7(4), 422-431
- Glenna, D.\* **Jana, A.\***, Xu, Q., Wang, Y., Meng, Y., Yang, Y., Neupane, M., Wang, L., Zhao, H., Qian, J., and Snyder, S. W. “Theoretical guidelines for activated carbon-based CO<sub>2</sub> adsorption material evaluation.” The Journal of Physical Chemistry Letters (2023): 14(47), 10693-10699. \* equal contribution.
- **Jana, A.**, Snyder, S. W., Crumlin, E. J., and Qian, J. “Integrated carbon capture and conversion: A review on C<sub>2+</sub> product mechanisms and mechanism-guided strategies.” Frontiers in Chemistry (2023): 11, 1135829
- **Jana, A.**, Kearney, L., Naskar, A., Grossman, J. C., and Ferralis, N. “Effect of methyl groups on formation of ordered or layered graphitic materials from aromatic molecules.” Small (2023): 19(43), 2302985
- Patil, J. J., Lu, Z., Zachman, M. J., Chen, N., Reeves, K. S., **Jana, A.**, Revia, G., MacDonald, B., Keller, B. D., Lara-Curzio, E., Grossman, J. C., and Ferralis, N. “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.**, Zhu, T., Wang, Y., Adams, J. J., Kearney, L., Naskar, A., Grossman, J. C., and Ferralis, N. “Atoms to Fibers: identifying novel processing methods in the synthesis of pitch-based carbon fibers.” Science Advances (2022): 8(11), eabn1905.
- **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.
- Patil, J. J.\* **Jana, A.\***, Getachew, B. A., Bergsman, D. S., Gariepy, Z., Smith, B. D., Lu, Z., and Grossman, J. C. “Conductive carbonaceous membranes: recent progress and future opportunities.” Journal of Materials Chemistry A (2021): 9(6), 3270-3289. \* equal contribution.

- **Jana, A.**, Sridar, S., Fries, S. G., Hammerschmidt, T., and Kumar, K. H. “Thermodynamic modelling of the Ni–Zr system.” *Intermetallics* (2020): 116, 106640.

## Invited Talks and Conferences

- **Jana, A.** “Nanoconfinement in metal/ligand electrocatalysts: how is it created and why does it reduce CO<sub>2</sub> efficiently?” Talk at Atomic, Molecular, and Optical Sciences (AMOS) seminar, December 2, 2025, LBNL, Berkeley, California.
- **Jana, A.** “Nanoconfinement in metal/ligand electrocatalysts: how is it created and why does it reduce CO<sub>2</sub> efficiently?” Invited Talk at UC Berkeley Bakar Institute of Digital Materials for the Planet (BIDMaP) Young Scholar Seminar, April 22, 2025, UC Berkeley, Berkeley, California.
- **Jana, A.** “Nanoconfined electrocatalysts for CO<sub>2</sub> reduction” Invited Talk at UC Merced Graduate Seminar series organized by Materials and Biomaterials Science and Engineering Graduate Program, September 16, 2024, UC Merced, Merced, California.
- **Jana, A.** “Explicit modeling of the solvent in electrocatalysis” Talk at Atomic, Molecular, and Optical Sciences (AMOS) seminar, December 5, 2023, LBNL, Berkeley, California.
- **Jana, A.**, Crumlin, E. J., and Qian, J. “Designing the nanoconfined microenvironment in metal/ligand catalysts for enhanced CO<sub>2</sub> electrochemical reduction” Oral and poster presentation at American Chemical Society Fall 2024; 2024 August 18-22; Denver, Colorado.
- **Jana, A.**, Qian, J., and Crumlin, E. J. “Creating the right microenvironment in metal/ligand catalysts at low potentials: a recipe for energy efficiency” 3-minute oral and Poster presentation at: 2nd Gerischer Electrochemistry Today Symposium; 2024 Aug 6-8; Colorado State University, Fort Collins, Colorado.
- **Jana, A.**, Crumlin, E. J., and Qian, J. “Nanoconfinement in metal/ligand electrocatalysts: how is it created and why does it reduce CO<sub>2</sub> efficiently?” Poster presentation at: West Coast Theoretical Chemistry 2024; 2024 May 5; Merced, California.
- **Jana, A.**, Qian, J., and Crumlin, E. J. “Impact of surface defects like vacancies and dopants on the design of energy-efficient Ag nanoparticle/ligand-based catalysts for electroreduction of CO<sub>2</sub>.” Poster presentation at: Materials Research Society Spring 2024; 2024 Apr 22-26; Seattle, Washington.
- **Jana, A.**, Shan, Y., Zhao, X., Fonseca, G. M., Jaugstetter, M., Yang, P., Salmeron, M., and Qian, J. “Explicit modeling of the solvent in electrocatalysis: a case study illuminating its effect on the catalyst structure.” Oral and poster presentation at: American Chemical Society Fall 2023; 2023 Aug 13-17; San Francisco, California.
- **Jana, A.**, Kearney, L., Naskar, A., Grossmann, J. C., and Ferralis, N. “Effect of methyl groups on crosslinking reactions in carbon-based systems.” Oral presentation at: American Chemical Society Spring 2023; 2023 Mar 26-30; Indianapolis, Indiana.

- **Jana, A.**, Bergsman, D. S., and Grossman, J. C. “Adsorption-based membranes for air separation using transition metal oxides.” Oral presentation at: American Chemical Society Spring 2022; 2022 Mar 20-24; San Diego, California.
- **Jana, A.**, Zhu, T., Wang, Y., Adams, J. J., Kearney, L., Naskar, A., Grossman, J. C., and Ferralis, N. “Atomistic modeling of carbon fibers made from pitch: insight into elastic modulus.” Oral presentation at: American Chemical Society Fall 2021; 2021 Aug 22-26; Atlanta, Georgia.
- **Jana, A.**, Fries, S. G., Hammerschmidt, T., and Kumar, K. H. *Ab initio* calculations of the intermetallics in the Ni-Zr system. Poster presented at: CALPHAD XLVI International conference; 2017 Jun 11-16; Saint-Malo, France.

## Teaching Experience

**Department of Materials Science and Engineering,  
Massachusetts Institute of Technology** Cambridge, USA

*Teaching Assistant* | Solid state chemistry Sep. – Dec. 2019

- Coordinated with Prof. Jeffrey Grossman and a team of ~20 teaching assistants in instructing ~500 undergraduate students
- Prepared and presented recitations, conducted office hours, and designed and graded exams

**Department of Metallurgical and Materials Engineering,  
Indian Institute of Technology Madras** Chennai, India

*Teaching Assistant* | Thermodynamics of Materials Aug. – Nov. 2016

- Assisted Prof. K. C. Hari Kumar in teaching 42 undergraduate (sophomore) students
- Designed assignments, conducted recitations, and evaluated exam papers

## Mentoring experience

- Hired and mentored an undergraduate summer intern working on simulating permeation of water through carbon-based nanoconfined structures (2024)
- Guided a graduate student on computational modeling of functionalized graphene for gas adsorption; published a paper together (2022-2023)
- Mentored an undergraduate intern transitioning to molecular dynamics simulations from experiments during the pandemic (2020)
- Helped undergraduate interns chosen for Mitacs Globalink with their project and stay in Canada (2016)
- Co-founded a community of materials science enthusiasts at IIT Madras; taught quantum mechanics informally to undergraduate peers (2015)

## Honors and Awards

- Winner of the three-minute lightning round talk at the 2nd Gerischer Electrochemistry Today Symposium; highlighted by RSC Materials (August 6, 2024)
- Research on the creation of nanoconfinement in metal nanoparticle/ligand-based electrocatalysts highlighted in **ALSNews** (May 1, 2024) and the **Berkeley Lab newsletter- Elements** (May 15, 2024)
- Recipient of a **DOE Office of Science Travel Award** for the 2nd Gerischer Electrochemistry Today Symposium
- Finalist in the **Berkeley Lab SLAM 2023**; interview featured in the **Berkeley Lab newsletter- Elements** (Nov 30, 2023)
- Research on identifying new ways to make carbon fibers out of refinery byproducts highlighted in **MIT News** (March 18, 2022) as well as other media outlets
- Recipient of the **S Anantharamakrishnan Memorial Prize** for the best dual degree academic record in the Department of Metallurgical and Materials Engineering, IIT Madras
- Recipient of the **Sri Satish Pai Prize** for the best academic record for the 3<sup>rd</sup> and 4<sup>th</sup> semesters in the Department of Metallurgical and Materials Engineering, IIT Madras
- One of the ~160 students from India selected for **DAAD-WISE** program for the year 2016
- One of the ~750 students from six countries selected for **Mitacs Globalink Research Internship** program for the year 2015
- Selected for Kishore Vaigyanik Protsahan Yojana (**KVPY**) scholarship 2012 with All India Rank of 613
- Placed in the **Top 1%** among 40000 students in the National Standard Examination in Physics, India, 2011

## Outreach experience

- Volunteered at the LBNL booth in the **Oakland Black Joy Parade**; helped the community know about opportunities at LBNL; aided children with viewing everyday objects under microscopes (Feb. 25, 2024, Feb. 23, 2025)
- Presented my research to eighth grade students as a part of a **Reverse Science Fair** to promote STEM awareness (Apr. 18, 2024, Dec. 10, 2024)
- Mentored undergraduate students in a workshop for “What to Expect in Grad School” organized by American Chemical Society Fall 2024, Denver (August 18, 2024)
- Volunteered as a job shadow host for high school students with underrepresented genders in STEM organized by **Science Accelerating Girls’ Engagement** at LBNL (June 11, 2024)

- Promoted STEM awareness as a **Role Model Volunteer** among elementary school girls of color from low-income families organized by Scientific Adventures for Girls (May 9, 2024)
- Volunteered for informal lunch talks with high school students (Mar. 20, 2024, Jan. 20, 2023)
- Supported career workshops for high school students in **Berkeley Lab Director's Apprenticeship Program** 2023-2024 (Mar. 16, 2024)
- Assisted with hands-on STEM activities with 6th graders in King Middle School (Feb. 28, 2024)

## Professional Service

- Editorial Board member of Discover Catalysis and Discover Surfaces journals
- Peer Reviewer for Nature Catalysis, Scientific Reports, ACS Omega, Journal of Reinforced Plastics and Composites, Water-Energy Nexus, and RSC Advances
- Chaired a session of the symposium– Electrocatalysis for Sustainable Energy: Fundamentals, Applications, and Perspectives in the American Chemical Society Fall 2023 conference held in San Francisco, California
- Session recorder for the session on Latest and Greatest from early career researchers at the 2nd Gerischer Electrochemistry Today Symposium (August 7, 2024)

## References

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