Asmita Jana

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Postdoctoral Researcher, Chemical Sciences Division
Lawrence Berkeley National Laboratory, Berkeley, CA

Research Interests

Computational Chemist with 7+ years of experience using Quantum Chemistry calculations (Density Functional Theory) and Molecular Dynamics for property prediction, materials discovery, and structure-to-function modeling in energy technology applications. Experience includes modeling interactions in ligand-based catalysts, reactions of organic molecules, and permeation of fluids through graphene membranes. 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 — Cambridge, USA
Ph.D. in Materials Science and Engineering — Sep 2017 – Aug 2022
GPA: 4.8/5
Advisor: Prof. Jeffrey C. Grossman
Thesis: Design of surface and bulk interactions: A computational approach to sustainable energy

Indian Institute of Technology Madras — Chennai, India
M.Tech. and B.Tech. in Metallurgical and Materials Engineering — Aug 2012 – Jul 2017
GPA: 9.63/10; Class topper
Advisor: Prof. K. C. Hari Kumar
Thesis: Thermodynamic optimization of the Ni-Zr system

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
- **Programming and software dev**: Python, C, C++, Fortran, MATLAB, Linux (Bash, Vim), HPC (slurm), NumPy, Matplotlib, Pandas
- **Visualization softwares**: VMD, Avogadro, Ovito, VESTA
- **Thermodynamic softwares**: Thermo-Calc, FactSage
- **Finite element analysis software**: ABAQUS
- **Graphic design and Typesetting**: Adobe Illustrator, LaTeX

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

Research Experience

Chemical Sciences Division, Berkeley, USA
Lawrence Berkeley National Laboratory

Machine learning potentials for catalytic properties
Jul. 2025 – Present

Postdoctoral Researcher | Advisors: Dr. Jin Qian

- Using Meta's Universal Model of Atoms (UMA) to evaluate the adsorption energies and other rate-determining properties of catalysts for the Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER) and compare them to the energies obtained using Density Functional Theory (DFT) calculations

Simulating nanoconfined solid N_2 within ice clusers
Jul. 2025 – Present

Postdoctoral Researcher | Advisors: Dr. Jin Qian, Dr. Jennifer Bergner

- Using ABCluster and subsequent DFT calculations to evaluate the structure and properties of solid N_2 confined within ice clusters; experimental efforts indicate altering chemical environment of solid N_2

Chemical reaction energy landscape in nanoconfinement
Feb. 2024 – Present

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

- Calculating the Gibbs free energies of the reaction intermediates in the CO_2 reduction to CO and hydrogen evolution reaction using DFT in nanoconfined interfaces with 2D confining surfaces and 3D organic ligand as confining species
- Preliminary results show enhanced stability of the reaction intermediates in ligand-confined microenvironment due to dipole interactions with ligand

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
- 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, Ruhr Universität Bochum Bochum, Germany

***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, Polytechnique Montréal Montréal, Canada

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- $BaCl_2$+BaF_2 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.**, 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: A blueprint for digitizing chemistry characterizations." Nature Computational Science (2025, accepted)
- 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_2 sorption." ACS Sustainable Chemistry and Engineering (2025): 13(16), 5974-5984
- 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_2 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 C2+ 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_2 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_2 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_2 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_2 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_2." 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 3rd and 4th 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

- Peer Reviewer for Nature Catalysis, Scientific Reports, ACS Omega, Water-Energy Nexus, and RSC Advances, 2024 onwards

- 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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