Krishnendu Mukherjee (Krish)

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Professional Summary

• Chemical Engineering Ph.D. candidate with interest in computational materials discovery and process optimization using molecular modeling, statistics, and data science.
• Performed successful and self-directed computational research in fields related to gas adsorption, machine learning, gas separation, and sensing with nanoporous materials.
• Communicated my research work to a wider audience by presenting at 4 national conferences, and published 5 papers in reputed journals.
• Expertise in simulating materials using scientific computational/modeling packages (RASPA, LAMMPS, ORCA etc.), and proficient in the use of programming and machine learning tools (python and Linux).
• Professional experience of 4+ years as an assistant manager in Indian oil corporation limited, leading the operation, process control, and maintenance for Hydrogen generation and Sulphur recovery units.

Education

• **University of Notre Dame, Notre Dame, IN** (Aug 2019 - Present)
Doctor in Philosophy, Chemical Engineering, *GPA 3.83/4.0*
• **State University of New York, Buffalo, NY** (Aug 2017 - June 2019)
Masters in Science, Chemical Engineering, *GPA 4.0/4.0*
• **National Institute of Technology, Durgapur, India** (June 2009 - June 2013)
Bachelors in Technology, Chemical Engineering, *GPA 8.11/10.0*

Professional Experience

Chemical and Biomolecular Engineering, University of Notre Dame, *Notre Dame, IN*
Advisor: Dr. Yamil Colón, Assistant Professor, University of Notre Dame (Oct 2019 - Present)
• Implemented an Active learning protocol (using Gaussian Process regressions) to predict methane and carbon dioxide adsorption in a Cu-BTC metal-organic framework (MOF) for a temperature-pressure phase space, and demonstrated a reduction of 97-98% of the total data requirement with comparable accuracy to high-fidelity monte carlo simulations.
Github: https://github.com/mukherjee07/Sequential-design-adsorption-for-small-molecules-in-MOFs
• Designed a Active learning workflow to predict gas mixture adsorption in MOFs (CO_2-CH_4, H_2S-CO_2, and Xe-Kr) saving 93 to 97% of the ground truth data while a prediction $R^2 \sim 1$.
• Developed an accuracy-based protocol as a stoppage criteria for the Active learning on gas mixture adsorption in MOFs for a pressure-mole fraction and also for pressure-mole fraction-temperature phase space (CO_2-CH_4, H_2S-CO_2, and Xe-Kr).
Github: https://github.com/mukherjee07/Active-Learning-for-multicomponent-adsorption-in-a-MOF
• Led and assisted an undergraduate student, Jack Gonzalez, to calculate selectivity of 30 gas mixtures (all combinations of CO_2, N_2, N_2O, O_2, CH_4, and H_2O) on the CoRE-MOF database (> 9000 structures), performed the structure-property analysis, and recommended MOF candidates for gas sensing.
• Simulated water vapor adsorption and density profiles on Idealized Carbon cylinders (ICC) and demonstrated the role of pressure, pore diameter, and electrostatics in influencing the hydrophilicity of ICCs.

Chemical and Biological Engineering, State University of New York, *Buffalo, NY*
Advisor: Dr. Johannes Hachmann, Associate Professor, SUNY Buffalo (March 2018 - Aug 2019)
• Designed a python and shell-based workflow on Linux to automate batch submission of computational chemistry calculations and extract properties of interest such as Single Point Energy, Atomic charges, Fukui Indices etc.
Github: https://github.com/mukherjee07/ORCA-project-Li-ion-battery-material-discovery

Assistant Manager(Production) at Indian Oil Corporation Limited (July 2013 - July 2017)
• Led operation team for Hydrogen Generation and Sulphur Recovery Unit at *Digboi Refinery* to achieve production targets with activities including emergency handling, maintenance, shutdown planning, process improvement etc.
• Effectively controlled and monitored process units by fine-tuning parameters within the advanced process control (APC) system, while also operating processes utilizing Yokogawa Distributed Control Systems (DCS) for enhanced efficiency and reliability.
• Implemented total productive maintenance (TPM) routines to proactively identify and prioritize critical areas for scheduled maintenance, including condensers, rorating equipment, and steam traps.

Publications

• Machine Learning and descriptor selection for the computational discovery of metal-organic frameworks. K Mukherjee, and YJ. Colón. *Molecular Simulation.* (2021)
DOI: https://doi.org/10.1080/08927022.2021.1916014
• Sequential Design of Adsorption Simulations in Metal-Organic Frameworks. K Mukherjee, AW Dowling, and YJ Colón. *Molecular Systems Design and Engineering.* (2022)
DOI: https://doi.org/10.1039/D1ME00138H
• Understanding structure-property relationships of MOFs for gas sensing through Henry's constants. J Gonzalez*, K. Mukherjee* and YJ Colón. *Journal of Chemical Engineering and Data.* (2022) (*shared first author) DOI: https://doi.org/10.1021/acs.jced.2c00443
• Active Learning for Adsorption Simulations: Evaluation, Criteria Analysis, and Recommendations for Metal–Organic Frameworks. Etinosa Osaro, K. Mukherjee, and YJ Colón. *Industrial & Engineering Chemistry Research.* (2023) DOI: https://doi.org/10.1021/acs.iecr.3c01589
• Active learning for efficient navigation of multi-component gas adsorption landscapes in a MOF. K Mukherjee, Etinosa Osaro, and YJ Colón. *Digital Discovery.* (2023)
DOI: https://doi.org/10.1039/D3DD00106G

Technical Skills and Awards

• **Programming**: Python (48 months), BASH (48 months), MATLAB (6 months), Gnuplot (6 months), Github (12 months), Jupyter (4 months), C++ (4 months), Pyomo (2 months).
• **Simulation**: ORCA (18 months), RASPA (24 months), LAMMPS (6 months), Gaussian (2 months), Zeo++ (2 months), Quantum-Espresso (2 months).
• **Research**: Monte Carlo simulations, Molecular Dynamics, Machine learning, Bayesian optimization, Quantum chemistry calculations.
• Notre Dame Graduate School Professional Development Award 2022.
• FOMMS Early Career researcher award by NSF.
• Travel award for Fundamental of Adsorption 14^{th} conference.
• Eilers graduate fellowship 2021 by ND Energy, University of Notre Dame.
• Secured an All India rank of 65 in **GATE** (Graduate Aptitude Test in Engineering), 2013 (99.60 %tile).

Leadership and Service

• Manuscript Reviewer for *ACS Applied Materials and Interfaces* and *Molecular Simulation* (4 reviews)
• Social Chair, Chemical Engineering Graduate Student Organization, *Notre Dame, IN* (April 2020-21)

References

• Prof. Yamil J. Colón, Assistant Professor, University of Notre Dame, email: ycolon@nd.edu
• Prof. Alexander W. Dowling, Assistant Professor, University of Notre Dame, email: adowling@nd.edu
• Prof. Johannes Hachmann, Associate Professor, University at Buffalo, email: hachmann@buffalo.edu