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

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)

• Designed an Active learning workflow to predict gas mixture adsorption in a MOF (with a diverse set of mixtures: CO_2-CH_4, H_2S-CO_2, and Xe-Kr) saving 93 to 97% of the ground truth data with a coefficient of determination, R^2 of ~ 1 compared with ground truth.
• Developed a perceived accuracy-based (PAC) protocol as a termination criteria for the Active learning on gas mixture adsorption for two set of features (pressure-mole fraction and pressure-mole fraction-temperature phase space).
• Established the efficiency of the AL-based model against IAST-based predictions (state-of-the-art theoretical model for mixture adsorption prediction) and shown close agreement with experimental data. Resulted in a publication in *RSC Digital Discovery* and informed an ongoing project on physics-informed active learning.
Github: https://github.com/mukherjee07/Active-Learning-for-multicomponent-adsorption-in-a-MOF

• 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 with a mean relative error under 2%.
• Demonstrated that Active learning for pure-components can reduce of 97-98% of the total data requirement with comparable accuracy to high-fidelity monte carlo simulations.
• Published the work in *RSC Molecular Systems Design and Engineering* and inspired another work on active learning for a diverse set of MOFs which was published in *ACS Industrial and Engineering Chemistry Research*. The work also served as a critical component of a successful NSF career award application.
Github: https://github.com/mukherjee07/Sequential-design-adsorption-for-small-molecules-in-MOFs.

• Led a project on sensor modeling with 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 crystal structures).
• Assisted in the MOF structure-property analysis, sorting out best candidate structure, and recommending MOF candidates for an all around binary gas sensor. Resulted in a publication with shared first author in *ACS Journal of Chemical Engineering and Data*.

• Simulated water vapor adsorption using monte carlo simulations in idealized carbon-based structures and demonstrated the role of charge configurations, pressure and pore diameter in adsorption.
• Performed density profiles, radial distribution function, and hydrogen bond network calculations to understand hydrophilicity of ICCs and water adsorption sites in the idealized structures. Also, resulted in a conference talk at *AIChE*.
Github: https://github.com/mukherjee07/Water-vapor-adsorption.

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 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, rotating equipments, reactors, burners, and steam traps.

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, Mathematical Modeling, Machine learning, Bayesian optimization, Quantum chemistry calculations.
• Notre Dame Graduate School Professional Development Award 2023.
• FOMMS Early Career researcher award by NSF.
• Notre Dame Graduate School Professional Development Award 2022.
• Travel award for Fundamental of Adsorption 14th 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)