Shivam Parashar

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Education

Rutgers University, New Brunswick, NJ — *Aug 2018-May 2024*
Doctor of Philosophy (Ph.D.) | Chemical and Biochemical Engineering — **GPA: 3.96/4**
Indian Institute of Technology Roorkee, Roorkee, UK, India — *Jul 2014-May 2018*
Bachelor of Technology (B.Tech.) | Chemical Engineering — **CGPA: 8.5/10**

Additional Training

Molecular Simulations (MolSim) Workshop — *Jan 2019*
University of Amsterdam, NL

Technical Skills

Computer Languages	C/C++, Python (NumPy, Pandas, Sklearn, SciPy, TensorFlow), Bash, MATLAB, Fortran, Git/GitHub, HTML, CSS, Unix/Linux
Software Packages	RASPA, LAMMPS, Towhee, Amber, CP2K, Gaussian, VMD, LIGGGHTS, SolidWorks, LaTeX, Jupyter Notebooks, Excel, Mathematica, Office Suite
Simulation Methods	Monte Carlo, Molecular Dynamics, Machine Learning, Density Functional Theory, Dissipative Particle Dynamics, Quantum and Ab initio methods
Laboratory	Design and execution of adsorption and absorption experiments

Publications

- **Parashar, S.**; Ravikovitch, P.; Neimark, A.V. *Molecular Modeling and Adsorption Characterization of Micro-Mesoporous Kerogen Nanostructures.* Energy & Fuels, **2022**, 36 (21), 13037-13049, DOI: 10.1021/acs.energyfuels.2c02876
- **Parashar, S.;** Zhu, Q.; Dantas, S.; Neimark, A.V. *Monte Carlo Simulations of Nanopore Compartmentalization Yield Fingerprint Adsorption Isotherms as a Rationale for Advanced Structure Characterization of Metal-Organic Frameworks*. ACS Appl. Nano Mater. **2021**, 4, 5, 5531-5540, DOI: 10.1021/acsanm.1c00937
- **Parashar, S.**; Jha, P. K. *Trends in pKa Values for polyprotic carboxylic acids. Chem. Phys.* arXiv **2020.** Preprint
- **Parashar, S.**; Lesnicki, D.; Sulpizi, M. *Increased Acid Dissociation at the Quartz/Water Interface.* J. Phys. Chem. Lett. **2018**, *9*, 2186-2189, DOI: 10.1021/acs.jpclett.8b00686

Conferences

- **Parashar, S.**; Ravikovitch P. I.; Neimark A. V. *Machine Learning Approach for Construction of Fingerprint Kernels for Pore Structure Characterization of Metal-Organic Frameworks*. AIChE Annual Meeting, Phoenix, Nov 16, 2022. **Oral Presentation.**
- **Parashar, S.**; Ravikovitch P. I.; Neimark A. V. *Adsorption based Pore Structure Characterization of Kerogen Fractions of Shales*. Fundamental of Adsorption Conference, Denver- Co, May 24, 2022. **Oral Presentation.**
- **Parashar, S.**; Ravikovitch P. I.; Neimark A. V. *Monte Carlo and Density Functional Theory for Pore Structure Characterization of Kerogen*. Molecular Simulations Workshop- NJIT, May 10, 2022. **Oral Presentation.**
- **Parashar, S.**; Ravikovitch P. I.; Neimark A. V. *Molecular Modeling and Adsorption Characterization of Micro-Mesoporous Kerogen Nanostructures*. AIChE Annual Meeting, Boston- MA, Nov 10, 2021. **Oral Presentation.**
- **Parashar, S.**; Dantas, S.; Venkatraman, S.; Ravikovitch P. I.; Neimark A. V., *Advanced Pore Structure Characterization of Crystalline and Amorphous Materials*. Webinar at University of Laval, Feb 04, 2022. **Oral Presentation.** Invited Speaker
- **Parashar, S.**; Ravikovitch P. I.; Neimark A. V. *Molecular Modeling and Adsorption Characterization of Micro-Mesoporous Kerogen Nanostructures*. AIChE Annual Meeting, Boston- MA, Nov 10, 2021. **Oral Presentation.**
- **Parashar, S.**; Venkatraman, S.; Dantas, S.; Neimark A.V. *Revealing Specifics of Gas Adsorption in Metal-Organic Frameworks from Compartmentalization of Isotherms*. AIChE Annual Meeting, Boston- MA, Nov 08, 2021. **Oral Presentation.**

- **Parashar, S.**; Venkatraman, S.; Dantas, S.; Neimark A.V. *Pore Level Compartmentalization of Adsorption Isotherms as a Rationale for Pore structure characterization of Metal-Organic Frameworks*. International Adsorption Society Invited Webinar, Aug 17, 2021**. Oral Presentation**. Invited Speaker
- **Parashar, S.**; Zhu, Q.; Dantas, S.; Neimark A.V. *Pore Level Decomposition of Adsorption Isotherms in Metal-Organic Frameworks*. IAS Twitter Conference, Dec 7-11, 2020. **Poster Presentation.** Best poster award
- **Parashar, S.**; Zhu, Q.; Dantas, S.; Neimark A.V. *Decomposition of Adsorption Isotherms to characterize Metal-Organic Frameworks*. AIChE Annual Meeting, San Francisco- CA, Nov 16, 2020. **Oral Presentation**.
- **Parashar, S.**; Zhu, Q.; Dantas, S.; Neimark A.V. *Decomposition of Adsorption Isotherms with respect to pore type in Metal-Organic Frameworks.* MolSim, Amsterdam- NL, Jan 9, 2020. **Poster Presentation**
- **Parashar, S.**; Dudawat, L.; Anand A. *Segregation of Non-Spherical Granular Particles in a Rotating Cylinder*. ACS on Campus, Indian Institute of Technology Roorkee, Feb 7, 2018. **Poster Presentation**. Best poster award

Relevant Coursework

Artificial Intelligence	Machine Learning and Statistics
Statistical Mechanics	Nanoscale Thermodynamics
Polymer Physics and Rheology	Computational Chemistry
Computational Physics	Multiscale Molecular Modeling
Introduction to College Teaching	Quantum Mechanics

Industrial Experience

Multiscale Modeling Intern | ExxonMobil, Annadale, NJ *Sep 2022-Present*

- Generated a realistic structure of amorphous organic material of shales using Molecular Dynamics. Proposed a multiscale approach to calculate pore volume, surface area and pore size distribution using Monte Carlo and Density Functional Theory

Academic Experience

Ph.D. Candidate and Research Assistant | Rutgers University, New Brunswick, NJ *Aug 2018-Pesent*

- **Supervised learning to predict adsorption:** Developed a Machine Learning model to predict adsorption in Metal-Organic Frameworks. The model identified promising materials for CO_2 storage
- **Unsupervised learning for compartmentalization:** Developed an unsupervised machine learning algorithm to calculate the fingerprint isotherms based on in-silico spatial distribution of adsorbate molecules at each pressures
- **Monte Carlo software development**: Developed a Grand Canonical Monte Carlo simulation software in C for adsorption of a monoatomic and triatomic gas molecule in slit and cylindrical pores
- **Modification of existing software**: Programed the gauge cell simulations in the existing software RASPA in C
- **Clean disorders in a structure**: Wrote an algorithm in python to clean site disorders in the MOF structure that intelligently removes partially occupied atoms and generates all non-equivalent configurations
- **Metal-Organic Framework (MOF) characterization:** Introduced a new method to calculate adsorption isotherms corresponding to individual pores of a MOF. The method computes sample crystallinity, degree of hydration, and pore accessibilities based on the experimental isotherm
- **Peptide Modeling:** Calculated the free energy of a peptide along a dihedral angle using Umbrella sampling in Amber

Computational Chemistry Intern | Johannes Gutenberg University Mainz, Germany *May-Jul 2017*

- Employed a combination of the electronic structure based Molecular dynamics and free energy perturbation approach to study quartz/water interface. Calculated the acidity of Pyruvic acid on the interface using the thermodynamics integration approach

Experiments and Modeling Intern | Indian Institute of Technology Madras, India *May-Jul 2016*

- Performed gas absorption experiments in microchannels and mill channels to monitor the dependence of mass transfer rate on the concentration and flow rates of the fluids. Developed a theoretical model to predict the diffusion coefficient of gas into the liquid

Research Assistant | Indian Institute of Technology Roorkee *Aug 2016-Jul 2018*

- Modeled pK_a of an oligomer of Acrylic acid in terms of conformation, tacticity, the number of carboxylic acid groups, and the charges on conjugated acid-base pair using Ab initio calculations
- Studied the segregation of binary mixture of particles of different shapes and sizes inside a rotating cylinder using Discrete Element Method simulations

Achievement and Awards

- **Best Poster award**, 1st International Adsorption Society Twitter Conference *2020*
- **Best Poster award**, ACS on Campus Indian Institute of Technology Roorkee *2018*
- **5th position**, ABU RoboCon India (National Robotic Competition) *2016*
- **First Runner-up**, Breach Wars (Robotic Competition) *2016*
- **First Runner-up**, Hobbies Club Techno-fest (Robotic Competition) *2015*

Leadership

- **Secretary**, Graduate Student Organization (2019-2021), *Rutgers University*
- **Research Mentor**, Aresty (2020), and Research-Intensive Summer Experience (2019), *Rutgers University*
- **Teaching Assistant**, Kinetics I and II (2022-21), Thermo (2019), Computational Methods (2018), *Rutgers University*
- **Mentor**, Student Mentorship Program (2017-2018), *Indian Institute of Technology Roorkee*