Mayank Agrawal

Postdoctoral Research Associate,
School of Engineering, Brown University,
184 Hope St, Box D, Providence RI 02912

(+1) 404 7847524
mayank_agrawal@brown.edu
www.mayankagr.com

Education

Jan 2015 – Dec 2019 **Ph.D., Chemical Engineering (Minor- Quantum Mechanics)**, *Georgia Institute of Technology (Georgia Tech)*, Atlanta. GPA: 3.9/4.0.

Jul 2009 – Jun 2014 **B.Tech & M.Tech (Dual Degree), Chemical Engineering**, *Indian Institute of Technology (IIT)*, Delhi. M.Tech GPA: 9.5/10.0, B.Tech GPA: 8.5/10.0.

Research Experience

Jan 2020 – present **Postdoctoral Research Associate**, *Brown University*, Providence, USA.
Advisor: Prof. Andrew Peterson
Research area: Electrocatalysis, Machine-learning, Fuel cells

Jan 2020 – present **Research Affiliate**, *Massachusetts Institute of Technology (MIT)*, Cambridge, USA.
Advisor: Prof. Adam Willard
Research area: Electrocatalysis, Rare Sampling Methods

Jan 2015 – Dec 2019 **Graduate Research Assistant**, *Georgia Institute of Technology (Georgia Tech)*, Atlanta, USA.
Advisor: Prof. David S Sholl
Thesis title: Computational Modeling of Adsorption of Complex Molecules in Metal-Organic Frameworks.

Jan 2013 – Jun 2014 **Graduate Research Associate**, *Indian Institute of Technology (IIT)*, Delhi, India.
Advisor: Prof. Kamal K. Pant
Thesis title: Catalytic steam reforming of model bio-oil over lanthanum doped Ni/CeO_2-ZrO_2

Computational Skills

Methods: Machine Learning (ML), Density Functional Theory (DFT), Monte Carlo (MC), Molecular Dynamics (MD)

Coding: Python, C++, Julia, Bash scripting, MATLAB, FORTRAN

Research Projects

Postdoctoral Projects

Method development to Utilize Machine Learning in Catalysis.

- Developing machine-learning algorithms to integrate theory and data science to accelerate catalyst developmen. Contributing to further develop Atomistic Machine-learning Package (*AMP*), an open source code designed to easily bring machine-learning to atomistic calculations.

Desorption of CO from Metal Surfaces in the Presence of Solvents.

- Implementing rare sampling methods such as Transition Path Sampling (TPS) and Umbrella Sampling to analyse the reaction coordinates in this multi-transition states system to predict free-energy surface
- Applying machine-learned potential to fast predict the thermodynamics and kinetics of the process.

Ph.D. Projects

Effect of Metal-Organic Frameworks (MOFs) Flexibility on the Adsorption of Gases.

- Developed an efficient and accurate methodology that combines ab-initio, Monte Carlo and Molecular Dynamics simulations to study the flexibility effects in MOFs on separation of industrial mixtures.
- Implemented the above methodology to study adsorptive separation of C_8 aromatics in flexible MIL-53.
- Extended the study to CoRE MOF database to explain the MOF flexibility effects on adsorption properties for 13 industrial gases.

Adsorption & Diffusion of Chemical Warfare Agents (CWAs) in MOFs.

- Derived non-bonded classical force-fields for CWAs and their simulants to predict their adsorption properties in MOFs.
- Performed high-throughput screening of MOFs using derived force-fields to find best performing MOFs for CWAs capture.
- Compared the adsorption and diffusion properties of CWAs with their simulants to address the question how accurately simulants are able to mimic CWAs' behavior in MOFs

Masters Project

Catalytic Steam Reforming of Model Bio-oil over La Doped Ni/CeO_2-ZrO_2.

- Synthesized Ni/CeO_2-ZrO_2 catalyst with different La metal percentage; carried out catalytic steam reforming using a fixed bed reactor to produce syn gas from model bio-oil.
- Modeled the kinetics of the steam reforming reaction to verify Langmuir-Hinselwood mechanism.

Publications

First Author Publications

1. **Agrawal, M.**, Han, R., Herath, D. & Sholl, D. S. "Does Repeat Synthesis in Materials Chemistry Obey a Power Law?" *Proceedings of National Academy of Sciences* 117 (2), 877-882 **(2020)**. doi:10.1073/*pnas*.1918484117
2. **Agrawal, M.**, Boulfelfel, S. E., Sava-Gallis, D. F., Greathouse, J. A. & Sholl, D. S. "Determining Diffusion Coefficients of Chemical Warfare Agents in Metal-Organic Frameworks." *The Journal of Physical Chemistry Letters* 10 (24), 7823-7830 **(2019)**. doi:10.1021/*acs*.*jpclett*.9*b*03119
3. **Agrawal, M.** & Sholl, D. S. "Effect of Flexibility on Adsorption in Nanoporous Materials at Dilute and Non-dilute Loadings." *ACS Applied Materials and Interfaces* 11 (34), 31060-31068 **(2019)**. doi:10.1021/*acsami*.9*b*10622
4. **Agrawal, M.**, Sava-Gallis, D. F., Greathouse, J. A. & Sholl, D. S. "How Useful are Common Simulants of Chemical Warfare Agents at Predicting Adsorption Behavior?" *The Journal of Physical Chemistry C* 122 (45), 26061-26069 **(2018)**. doi:10.1021/*acs*.*jpcc*.8*b*08856
5. **Agrawal, M.**, Bhattacharyya, S., Huang, Y., Jayachandrababu, K. C., Murdock, C. R., Bentley, J. A., Rivas-Cardona, A., Mertens, M., Walton, K. S., Sholl, D. S. & Nair, S. "Liquid Phase Multicomponent Adsorption and Separation of Xylene Mixtures by Flexible MIL-53 Adsorbents." *The Journal of Physical Chemistry C* 122 (1), 386-397 **(2018)**. doi:10.1021/*acs*.*jpcc*.7*b*09105

Co-Author Publications

6. Bingel, L. W., Chen, A., **Agrawal, M.** & Sholl, D. S. "Experimentally-Verified Alcohol Adsorption Isotherms in Nanoporous Materials from Literature Meta-analysis." *Journal of Chemical & Engineering Data* 65 (10) 4970-4979 **(2020)**. doi:10.1021/*acs*.*jced*.0*c*00598
7. Agrawal, A., **Agrawal, M.**, Suh, D., Fei, S., Alizadeh, A., Ma, Y., Matsuda, R., Hsu, W. & Daiguji, H. "Augmenting the Carbon Dioxide Uptake and Selectivity of Metal-Organic Frameworks by Metal Substitution: Molecular Simulations of LMOF-202" *ACS Omega* 5 (28), 17193-17198 **(2020)**. doi:10.1021/*acsomega*.0*c*01267
8. Agrawal, A., **Agrawal, M.**, Donguk, S., Yunsheng, M., Matsuda, R., Endo, A., Hsu, W. & Daiguji, H. "Molecular Simulation Study on the Flexibility in the Interpenetrated Metal-Organic Framework LMOF-201 Using Reactive Force Field." *Journal of Material Chemistry A* 8, 16385-16391 **(2020)**. doi:10.1039/*c*9*ta*12065*c*
9. Park, J., **Agrawal, M.** Sava-Gallis, D. F., Greathouse J. A. & Sholl, D. S. "Impact of Intrinsic Framework Flexibility for Selective Adsorption of Sarin in Non-Aqueous Solvents using Metal-Organic Frameworks." *Physical Chemistry Chemical Physics* 22, 6441-6448 **(2020)**. doi:10.1039/*c*9*cp*06788*d*

Talks & Posters

Conference Oral Talks

- 2019 Gordon Research Seminar (GRS) on Nanoporous Materials and Their Applications, Andover, New Hempshire, Aug 2019
  [One of 10 abstracts selected out of 65 for oral presentations at GRS]
- 2018 AIChE Annual Meeting, Pittsburgh, Pennsylvania, Oct 2018
- Annual ChBE Graduate Colloquium, Georgia Tech, Atlanta, Aug 2018
- 2017 AIChE Annual Meeting, Minneapolis, Minnesota, Oct 2017
- ChBE Graduate Research Symposium, Georgia Tech, Atlanta, Feb 2017

Conference Posters

- 2019 Gordon Research Conference (GRC) on Nanoporous Materials and Their Applications, Andover, New Hempshire, Aug 2019

Invited Talks

- Indian Institute of Technology (IIT) Bombay, Chemical Engineering, Jan 2019
- Indian Institute of Technology (IIT) Madras, Chemical Engineering, Jan 2019
- Indian Institute of Technology (IIT) Kanpur, Chemical Engineering, Jan 2019
- The International Institute of Information Technology (IIIT) Hyderabad, Natural Sciences, Jan 2019

Participation

- Vaishwik Bharatiya Vaigyanik Summit (VAIBHAV), Oct 2020

Teaching Experience

2018–2019 **Teach2Teaching Certificate Recipient**, *Center for Teaching and Learning*, Georgia Tech.
The program is designed to prepare Georgia Tech graduate students and postdocs for college teaching positions.
- Learnt theories of pedagogy that support effective teaching and learning in higher education
- Applied effective teaching methods by **co-teaching** "statistical thermodynamics" grad level course with Dr. Carson Meredith as a faculty mentor

2015–2016 **Graduate Teaching Assistant**, *Chemical Engineering*, Georgia Tech.
Courses: Chemical Engineering Thermodynamics, Unit Operations Lab

2014 **Teaching Faculty**, *Physical Chemistry*, JKs Academy, Mathura, India.

2012-2014 **Teaching Assistant**, *Chemical Engineering*, IIT Delhi.
Courses: Chemical Reaction Engineering, Heterogeneous Catalysis and Catalytic Reactors

Awards

2013 **Director's Merit Award**, for being in top 7% students, IIT Delhi.

2013 **MHRD Scholarship**, for securing All India Rank 104 amongst 15000+ in GATE.

Referee Experience

2018–present **Peer Reviewer**, *Have independently reviewed more than 15 journal papers.*
Journal of American Chemical Society(JACS), Langmuir, The Journal of Physical Chemistry C (JPCC) Physical Chemistry Chemical Physics (PCCP), RSC Advances, Journal of Material Chemistry A (JMCA)

Industrial Experience

2017 **Graduate Summer Intern**, *HyCO R&D*, Praxair Inc, Tonawanda, NY, USA.
Developed a gPROMS based PSA process for syn-gas purifier to replace conventional technology. Analyzed the feasibility of the new process and proposed a cost effective model for two-layer packed bed reactor to achieve desired product purity and high recovery.

2012 **Undergraduate Summer Intern**, Omnova Solutions Inc., Ankleshwar, Gujarat, India.
Conducted a thorough investigation of the recovery unit in the Nitrile Butadiene Rubber Plant to find the causes of high monomer wastage. Proposed a design of the recovery tower that reduces butadiene waste by 30%.

Referenes

Available on Request