

Mayank Agrawal

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Education

- Jan 2015– Dec 2019 **Ph.D., Chemical Engineering (Minor in Quantum Mechanics), Georgia Institute of Technology (Georgia Tech), Atlanta.** GPA: 3.9/4.0.
Thesis title: Computational Modeling of Adsorption of Complex Molecules in Metal-Organic Frameworks.
Advisor: Prof. David S Sholl
- Jul 2009– Jun 2014 **B.Tech and M.Tech, Chemical Engineering, Indian Institute of Technology (IIT), Delhi.**
M.Tech GPA: 9.5/10.0, B.Tech GPA: 8.5/10.0.
Thesis title: Catalytic steam reforming of model bio-oil over lanthanum doped Ni/CeO₂-ZrO₂

Research Experience

- Ph.D. Projects **Effect of Metal-Organic Frameworks 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 C₈ 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/CeO₂-ZrO₂.**
- Synthesized Ni/CeO₂-ZrO₂ 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.
- Data Science Projects **Course: Data Analytics for Chemical Engineers.**
- Developed machine learning models to predict bandgap formation energy of transparent semi-conductors using a DFT generated database.
- Course: Computational Problem Solving.**
- Created a Bitcoin software protocol in C to gain a deeper understanding of Bitcoin networks.

Computational Skills

- Atomistic Process Coding Density Functional Theory (DFT), Monte Carlo (MC), Molecular Dynamics (MD)
ASPEN, HYSYS, ANSYS FLUENT
Python, C, Bash scripting, MATLAB, FORTRAN

Peer Reviewing Activities

2018–present **Reviewer**, *Royal Society of Chemistry*, Have reviewed 5 journal papers.

2017–present **Reviewer**, *American Chemical Society*, Have reviewed 4 journal papers.

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

Work Experience

2017 **Graduate Summer Intern**, *HyCO R&D*, Praxair Inc, Tonawanda, NY.

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.

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.

Publications & Talks

First-author Journal Articles.

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* (Accepted). 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.jpcclett.9b03119
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.9b10622
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.8b08856
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.7b09105

Co-author Journal Articles.

1. 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." (**Submitted**)
2. 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." (**Submitted**)

Conference Talks.

1. **Agrawal, M.** & Sholl, D. S. "Effect of Intrinsic Framework Flexibility on Adsorption Properties in Metal-Organic Frameworks: A Computational Exploration" *Gordon Research Seminar on Nanoporous Materials and Their Applications*. Andover, NH (2019)
[One of 10 abstracts selected out of 65 for oral presentations at GRS]
2. **Agrawal, M.**, Sava-Gallis, D.F., Greathouse, J.A. & Sholl, D. S. "Computational Screening of Metal-Organic Frameworks for Adsorption of Organophosphate Chemical Warfare Agents." *AIChE Annual Meeting*. Pittsburgh, PA (2018)
3. **Agrawal, M.**, Sava-Gallis, D.F., Greathouse, J.A. & Sholl, D. S. "Transferability of Adsorption Properties between Chemical Warfare Agents and Their Simulants." *Annual ChBE Graduate Colloquium*, Georgia Institute of Technology, Atlanta GA (2018)
4. **Agrawal, M.**, Bhattacharyya, S., Rivas-Cardona, A., Mertens, M., Walton, K. S., Nair, S. & Sholl, D. S. "Framework Flexibility Driven Adsorptive Separation of C₈ Aromatic Isomers in Metal-Organic Frameworks: A Computational Exploration." *AIChE Annual Meeting*. Minneapolis, MN (2017)
5. **Agrawal, M.**, Bhattacharyya, S., Rivas-Cardona, A., Mertens, M., Walton, K. S., Nair, S. & Sholl, D. S. "Effect of Breathing in MIL-53 on Adsorption of C₈ Aromatic Isomers." *ChBE Graduate Research Symposium*, Georgia Institute of Technology, Atlanta GA (2017)

Poster Presentations.

1. **Agrawal, M.** & Sholl, D. S. "Effect of Intrinsic Framework Flexibility on Adsorption Properties in Metal-Organic Frameworks: A Computational Exploration" *Gordon Research Conference on Nanoporous Materials and Their Applications*. Andover, NH (2019)

Invited Talks.

1. **Agrawal, M.** & Sholl, D.S. "Effect of Intrinsic Framework Flexibility on Adsorption Properties of MOFs at Low and High Loadings."
 - Indian Institute of Technology (IIT) Bombay, Mumbai, India (January, 2019)
 - Indian Institute of Technology (IIT) Madras, Chennai, India (January, 2019)
 - Indian Institute of Technology (IIT) Kanpur, Kanpur, India (January, 2019)