Mayank Agrawal

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Education

2015–present (Nov 2019 expected) — **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

2009–2014 — **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/CeO_2-ZrO_2

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 of 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.

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 — Density Functional Theory (DFT), Monte Carlo (MC), Molecular Dynamics (MD)

Process — Aspen, Hysys, Ansys Fluent

Coding — Python, C, Bash scripting, Matlab, Fortran

Publications & Talks

Journal Articles.

1. **Agrawal, M.**, Sava-Gallis, D. F., Greathouse, J. A. & Sholl, D. S. "Diffusion of Chemical Warfare Agents and Simulants in Nanoporous Materials." **(Under Preparation)**.

2. **Agrawal, M.** & Sholl, D. S. "Effect of Flexibility on Adsorption in Nanoporous Materials at Dilute and Non-dilute Loadings." **(Submitted)**.

3. **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:$10.1021/acs.jpcc.8b08856$

4. **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:$10.1021/acs.jpcc.7b09105$

Presentations.

1. **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)

2. **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)

3. **Agrawal, M.**, Bhattacharyya, S., Rivas-Cardona, A., Mertens, M., Walton, K. S., Nair, S. & Sholl, D. S. "Framework Flexibility Driven Adsorptive Separation of C_8 Aromatic Isomers in Metal-Organic Frameworks: A Computational Exploration." *AIChE Annual Meeting*. Minneapolis, MN (2017)

4. **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 C_8 Aromatic Isomers." *ChBE Graduate Research Symposium*, Georgia Institute of Technology, Atlanta GA (2017)

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 (2019)

2. **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) Madras. Chennai, India (2019)

3. **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) Kanpur. Kanpur, India (2019)

Peer Reviewing Activities

2018–present   **Reviewer**, *Royal Society of Chemistry*, Have reviewed 1 journal paper.

2017–present   **Reviewer**, *American Chemical Society*, Have reviewed 3 journal papers.

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.

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

References

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