



# Dr. Abdul Sami

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**Website:** <https://scholar.google.com/citations?hl=en&user=2FHvU98AAAAJ>

## ABOUT ME

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### Strength Area:

Expert In: Programming: (*Python*), Machine Learning Techniques (*Supervised and unsupervised learning*), and Molecular Dynamics Simulation (*DFT & Monte Carlo*).

Experienced In: Data platforms: (MATLAB), AI/ML tools: (Jupyter Notebook)

Research area: CO<sub>2</sub> capture and utilization.

### Synopsis:

- My *doctoral work* focused on the synthesis of amine-functionalized polymer aerogel for CO<sub>2</sub> capture, and DFT/Monte Carlo molecular dynamics for insight into the molecular interactions and potential for industrial-scale CO<sub>2</sub> capture.
- *Published* 13 JCR Q1/Q2 articles related to AI/ML modeling, CO<sub>2</sub> capture and molecular dynamics,
- *Currently developing* six (6) AI/ML data driven models for petroleum industry application with PETRONAS funding.
- *Wrote five grant proposals* on integrating AI/ML for the petroleum industries.

## QUALIFICATIONS

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### Chemical Engineering

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- **PhD** in Chemical Engineering, 2025, Universiti Teknologi PETRONAS, Malaysia.
- **Master's** in Chemical Engineering, 2016, NED University of Engineering & Technology, Pakistan.
- **Bachelor's** in Chemical Engineering, 2013, Dawood College of Engineering & Technology, Pakistan.

## RESEARCH AND PROJECT EXPERIENCE

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### 2024-2025

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Universiti Teknologi PETRONAS, Malaysia

1. Currently **developing AI/ML models** for six (6) petroleum industry projects funded by PETRONAS (Ongoing).
2. **Dissertation Title:** *Initiator-Free Synthesis and Optimization of Amine-Impregnated Polymeric Aerogel Using Electron Beam Radiation for CO<sub>2</sub> Capture*. This innovative approach eliminates the need for chemical initiators, presenting a greener and more sustainable synthesis route in polymer processing. Results were published in the Q1 Journals.
3. **Project Title:** *Molecular dynamics simulation study on the effect of crosslinker concentration on polymer aerogel properties and its CO<sub>2</sub> adsorption*. Molecular dynamics provides valuable insights into their structural properties, molecular interactions, adsorption performance, and potential for industrial-scale CO<sub>2</sub> capture. Results were published in the Scopus journal.
4. **Project Title:** *Synthesis of Amine-Functionalized Fly Ash-Infused Polymeric Hydrogel for H<sub>2</sub>S Removal and Validation Using Molecular Dynamic Simulation*. Results were published in the Journal of Applied Polymer Science.

## TEACHING EXPERIENCE

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FEB 2016 – CURRENT

### Lecturer

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Department of Chemical Engineering, NED University of Engineering and Technology, Pakistan.

- **Delivered lectures** and tutorials for undergraduate courses, including Heat and Mass Transfer, Fluid Mechanics, Environmental Pollution and Control, Materials Science, and Engineering.
- **Conducted laboratory** sessions and provided hands-on training on Aspen Hysis, Materials Studio, and Design of Experiments for engineering simulations.
- **Mentored undergraduate** students, guiding them in high-impact research article writing, conference presentations, and industrial job-hunting tips.
- **Supervised final-year projects** on CO<sub>2</sub> capture and utilization, upstream oil-water separation, continuous catalyst regeneration process, and membrane synthesis for environmental applications.
- **Led industrial visits:** LOTTE Pakistan PTA, Pakistan Steel Mills, BYCO oil refinery.

## ● INDUSTRIAL EXPERIENCE

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### Process Engineer

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1. **Tufail Chemical Industries (Nov 2015-Feb 2016 ):** Dealing with the production of Linear Alkyl Benzene Sulfonic Acid (LABSA) using gas-liquid phase reaction on a falling film reactor.
2. **Gatron Industries Limited (Nov 2013-Feb 2015):** Deals in virgin PET Resin & Polyester resin & Yarn, having annual production using 5 in series CSTR reactors of 232000 tons per annum, ISO 9001, 14001 & 22000 Certified.
3. **Gamalux Private Limited (May 2013-Nov 2013):** Dealed in Distilled Fatty Acids. Gained in-depth knowledge of fatty acid production under high pressure of up to 30 bar and vacuum distillation processes.

## ● PUBLICATIONS

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### 2025-2023

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#### Published Papers:

1. A. Bari, W. Ahmed, M. Waqas, S. Mansoor, A. Hayat, **A Sami** "AI-Driven Optimization of Chemical Consumption in Oil Pipelines", *OnePetro*, Doi 10.2118/229206-MS.
2. W. Jusoh, M. Omar, **A. Sami**, K. Bingi, R. Ibrahim "Crude Oil Yield Estimation: Recent Advances and Technological Progress in Oil Refining Industry", *Sensor*, 2025, <https://doi.org/10.3390/s25175511>.
3. **A. Sami**, N. Ekmi, K.Johari, F. Hilmi, N. Osman, M. Ghani, & A. Shaan "Optimization study of an amine loaded fly ash based stable aerogel for enhanced CO<sub>2</sub> capture," *Polymer (Guildf)*., 2024,(**Q1: IF 4.1**), [doi: 10.1016/j.polymer.2024.127600](https://doi.org/10.1016/j.polymer.2024.127600).
4. **A. Sami**, K. Johari, F. F. Hilmi, M. Rashid, & N. Ekmi, "A new initiators-free technique for synthesizing stable amine-impregnated polymeric aerogel using electron beam radiation for CO<sub>2</sub> capture," *Polymer (Guildf)*., 2024, (**Q1: IF 4.1**), [doi: 10.1016/j.polymer.2024.126987](https://doi.org/10.1016/j.polymer.2024.126987).
5. **A. Sami**, N. Ekmi, K.Johari, M.Rashid, M. Ghani, A. Shaan, A.S. Khan "Development of an amine-impregnated polymer aerogel for CO<sub>2</sub> capture," *Colloids Surfaces A Physicochem*, 2024, (**Q1: IF 4.9**), [doi: 10.1016/j.colsurfa.2024.133778](https://doi.org/10.1016/j.colsurfa.2024.133778).
6. M. Awais Ali, S. Shah, M.Karim, S. Moiz, H.Farooq, A. Habib, **A. Sami** "State-of-the-Art Membrane Solutions for Direct Air Carbon Capture (DACC): An Overview on the Current Status and Future Directions" 2025, (**Q1: IF 5.3**) <https://doi.org/10.1021/acs.energyfuels.5c00793>
7. S. F. A. Shah, N. Ekmi, K. Johari, M Ghani, **A. Sami**" Synthesis of Amine-Functionalized Fly Ash-Infused Polymeric Hydrogel for H<sub>2</sub>S Removal and Validation Using Molecular Dynamic Simulation", *Journal of Applied Polymer Science*, 2025, (**Q1: IF 2.8**) <https://doi.org/10.1002/app.57341>.
8. M.Rashid, A. Shaan, R. Steven, **A. Sami**, S. Waqas, Z Noor Ahmad "Efficient Mercury Removal from Wastewater via Carbonized Inverse Vulcanized Copolymers", *ACS ES&T Water*, 2025, (**Q1: IF 4.3**) <https://doi.org/10.1021/acsestwater.5c00030>.
9. S. A. Ali, I. Hamza, S.Malik, A. Karim, F. Ahmad, M. Ahmad, K. Habib, S. Shah, **A. Sami**, Z. Laghari, A. Qudoos" Review on the Role of Electrofuels in Decarbonizing Hard-to-Abate Transportation Sectors: Advances, Challenges, and Future Directions", *Energy & Fuels*, 2025, (**Q1: IF 5.3**) <https://doi.org/10.1021/acs.energyfuels.4c06185>.
10. A. Shaan, M. Rashid, L. Qomariyah, J. W. Lim, **A. Sami**, and M. Ayoub, "Heavy metal sequestration from wastewater by metal-organic frameworks: a state-of-the-art review of recent progress," *Environ. Sci. Pollut. Res.*, 2024, (**Q1: IF 5.8**), [doi: 10.1007/s11356-024-33317-7](https://doi.org/10.1007/s11356-024-33317-7).
11. A. Shaan., M. Rashid, Z. Alothman, W. Ammara, A. Aljuwayid, S. Rabia, A. Amin, **A. Sami** "Amine-Decorated Methacrylic Acid-based Inverse Vulcanized Polysulfide for Effective Mercury Removal from Wastewater," *ACS Omega*, 2024,(**Q1: IF 4.1**), [doi: 10.1021/acsomega.3c08361](https://doi.org/10.1021/acsomega.3c08361).
12. A. Shaan, M. Rashid, A. Amin, A. Mohaira, Y. Yoshiaki, **A. Sami**, A. Hamad "The predictive machine learning model of a hydrated inverse vulcanized copolymer for effective mercury sequestration from wastewater," *Sci. Total Environ.*,(**Q1: IF 8.2**), [doi: 10.1016/j.scitotenv.2023.168034](https://doi.org/10.1016/j.scitotenv.2023.168034).
13. A. Shaan, M. Rashid, S. Rabia, W. Ammara, **A. Sami**, A. Hamad "Synthesis and performance evaluation of slow-release fertilizers produced from inverse vulcanized copolymers obtained from industrial waste †," *RSC Adv.*, 2023, (**Q1: IF 8.2**), [doi: 10.1039/d3ra00256j](https://doi.org/10.1039/d3ra00256j).

## ● CONFERENCES AND SEMINARS

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### 2025-2023

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1. **A. Sami**, K. Johari, F. Hilmi, S. Farman, N. Ekmi, Molecular dynamics simulation study on the effect of crosslinker concentration on polymer aerogel properties and its CO<sub>2</sub> adsorption, *Materials Research Proceedings* **53**, 322-333, (2025).
2. S. Farman, N. Ekmi, Johari K. Johari, M.G.S.Musliha, **A.Sami**, Optimization of fly ash-g-polyacrylic acid hydrogel via response surface methodology for improved amine loading capacity, *Materials Research Proceedings*, **53**, 146-154, (2025)

3. **A. Sami**, N. Ekmi, K. Johari, N. Osman, M. Ghani, F. Ullah, S.M. Tariq "Modeling Aerogels for CO<sub>2</sub> Capture: Insights into Structure and Adsorption Dynamics" (2024), *Proceeding of AMPE*.
4. M. Ghani, R. Kumeresan, N. Ekmi, M.A. Marzuki, **A. Sami**, Farah Najihah Azleen, Fly ash grafted poly (acrylic acid-co-acrylamide) composite hydrogel as the carbon dioxide adsorbent, *AIP Conference Proceedings* (2024).

## ● HONOURS AND AWARDS

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### 2025-2023

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1. Participating in a technical talk on "Machine Learning Applications In Petroleum Engineering" organized by SPE-UTP-SC.
2. Delivered a one-day hybrid hands-on training session on Origin Pro software in 2025. Organised by AISPC, Universiti Teknologi PETRONAS (UTP), Malaysia.
3. Participated in 3MT Competition (PhD Category) in 2025. Organised by Centre for Graduate Studies (CGS), Universiti Teknologi PETRONAS (UTP), Malaysia.
4. Was nominated for the publication achievement recognition award for Q1/Q2 journal articles in 2024. By the Centre for Graduate Studies (CGS), Universiti Teknologi PETRONAS (UTP), Malaysia.
5. Won the best oral presentation award on "modeling and simulation," by Monash University, 2023.
6. Won a silver medal in "Penang International Invention, Innovation, and Design" by Universiti Teknologi MARA, Malaysia, 2023.
7. Secured top position in bachelor final exams at Dawood College of Engineering and Technology, 2013.

## ● REFERENCES

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### Dr. Nurul Ekmi Rabat

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*(PhD Supervisor)*

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### Dr Farah Fadzehah Binti Hilmi

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