

# Malik Waqar Arshad

PhD. Candidate, University of Science and Technology (UST)  
Computational Chemist | Chemical Engineer

✉ chemcoms@kRICT.re.kr  
☎ (+82)10-2897-0863  
🏠 126-4 Sinsoeng-dong, Youseng-gu,  
Daejeon (34116), South Korea

 [Google Scholar](#)  [LinkedIn](#)  [ResearchGate](#)

## Biography

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Malik Waqar Arshad is a Chemical Engineer with 10 years of experience in the Industrial, academia, and R&D division. Before joining the University of Science and Technology (UST) and Korea Research Institute of Chemical Technology (KRICT), South Korea as a graduate researcher for his PhD studies, he served a couple of years in the Chemical Industry and 5 years at Dhofar University, Oman as a laboratory engineer and established Chemical Engineering Laboratories where he gains a vast range of lab development experience and also did many R&D projects topics including corrosion, nanoparticle synthesis, diesel quality improvement, bio-cellulose formation, water & wastewater treatments. Currently, he is working on heterogeneous catalysis, DFT calculation, C1 chemistry, microkinetic modelling and using machine learning (ML) tools for the development of complex reaction mechanisms.

## Education

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Aug 2022 **University of Science and Technology (UST), South Korea**  
Mar 2018 PhD in Chemical Engineering (Computational Catalysis)  
Academic Supervisor: Dr Seok Ki Kim & Dr Iljeong Heo

PhD Thesis Title: Catalyst design for CO-assisted NO<sub>x</sub> reduction using mechanistic and microkinetic modelling.

Feb 2012 **COMSATS University Islamabad, Lahore Campus, Pakistan**  
Mar 2008 B.S. in Chemical Engineering (Oil & Gas)

## Research Experience

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Present **C1 Gas and Carbon Convergent Research Center, UST-KRICT, South Korea**  
Mar 2018 Computational Catalysis (DFT), DeNO<sub>x</sub>, CO<sub>2</sub> Conversion, Microkinetic Modeling, Machine Learning

Feb 2018 **Dhofar University, Sultanate of Oman**  
Jan 2013 Reaction Engineering Lab, Separation Process Technology Lab, Biotechnology Lab, Fuel Cell Lab, Fluid Mechanics Lab, Water & wastewater Treatment Lab.

## Scholarships and Awards

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Mar 2018 **UST-KRICT Graduate Research Fellowship**  
Graduate research fellowship, awarded to students at UST-KRICT, which provides support towards stipend and research costs for MS and PhD in Chemical Engineering.

Feb 2018 **Best Service Award**  
In the recognition for the development of Chemical Engineering Laboratories at Dhofar University, Sultanate of Oman.

## Publications

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### Peer Review

1. **A first-principles understanding of the CO-assisted NO reduction on the IrRu/Al<sub>2</sub>O<sub>3</sub> catalyst under O<sub>2</sub>-rich conditions**  
**M.W. Arshad**, D.H. Kim, Y.W. You, S.M. Kim, I. Heo and S.K. Kim  
*Catal. Sci. Technol.*, **2021**, *11*, 4353-4366.
2. **Unraveling the origin of extraordinary lean NO<sub>x</sub> reduction by CO over Ir-Ru bimetallic catalyst at low temperature**  
Y.W. You, Y.J. Kim, J.H. Lee, **M.W. Arshad**, S.K. Kim, S.M. Kim, H. Lee, L.T. Thompson and I. Heo  
*Appl. Catal. B*, **2021**, *280*, 119374
3. **Unraveling the role of cobalt in the direct conversion of CO<sub>2</sub> to high-yield liquid fuels and lube base oil**  
H. Jo, M.K. Khan, M. Irshad, **M.W. Arshad**, S.K. Kim and J. Kim  
*Appl. Catal. B*, **2022**, *305*, 121041

## Under Process

1. **A study of particle size and metal-support interaction effects on Ir-Ru alloy supported on Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> for CO-assisted NO reduction in O<sub>2</sub>-rich condition**  
**M.W. Arshad**, Y.W. You, I. Heo and S.K. Kim
2. **In silico catalyst screening of CO-assisted NO reduction by using first-principle microkinetic modelling**  
**M.W. Arshad**, I. Heo and S.K. Kim
3. **NO reduction by CO over the NiO<sub>x</sub>/CeO<sub>2</sub> catalyst: A mechanistic insight**  
T.J. Kim, **M.W. Arshad** and S.K. Kim
4. **Study of Selective Reverse Water-Gas Shift Reaction over Pt/Na-Zeolite catalyst by Operando DRIFTS**  
S. Kim, **M.W. Arshad** and S.K. Kim

## Conference Contribution

1. **Synthesis and Characterization of Metal Oxide Nanomaterials for Advanced Energy Applications**  
M.W. Ahmad, **M.W. Arshad**, M. Ul-Islam, G.H. Lee  
Conference on Energy Challenges in Oman, ECO'2015
2. **Bio-ethanol from waste sources: A renewable energy source**  
M. Ul-Islam, M.W. Ullah, S. Khan, M.W. Ahmad, **M.W. Arshad**  
Conference on Energy Challenges in Oman, ECO'2015
3. **IrRu bimetallic alloy for the low- temperature NO reduction using CO**  
**M.W. Arshad**, Y.-W. You, I. Heo and S.K. Kim  
27th North American Catalysis Society Meeting, 2021 (Abstract Submitted)

## Teaching Experience

### Dhofar University, Sultanate of Oman

Fall	2017	<b>CHEE 270L: Fluid Mechanics Laboratory</b>
Spring	2013	The laboratory covers experiments that include the basic principles of fluid mechanics. The course helps students to combine elements of theory and practice.
		<b>CHEE 311L: Reactive Process Engineering Laboratory</b>
		The laboratory covers exercises in the design, operation and implementation of various types of simple chemical reactors.

### **CHEE 411L: Separation Processes Laboratory**

The laboratory covers exercises in techniques and instrumentation in separation processes.

### **CHEE 441L: Biotechnology Laboratory**

The laboratory covers exercises in techniques and instrumentation in biotechnology.

### **CHEE 476L: Chemical Reactor Design Laboratory**

The laboratory covers exercises in advanced chemical reactor design.

### **CHEE 487: Fuel Cell Laboratory**

The laboratory covers modern techniques for the design and assessment of fuel cells, and the deployment in hybrid electric systems.



## **Employment History**

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Present  
Mar 2018

### **Korea Research Institute of Chemical Technology (KRICT), South Korea**

Graduate Researcher at C1 Gas and Carbon Convergent Research Center.

#### **Responsibilities & Duties:**

- Density functional theory (DFT) calculation using VASP software.
- Working on the reaction mechanism of DeNOx and CO<sub>2</sub> Conversion system.
- Microkinetic Modeling for the complex reaction networks.
- Applying Machine Learning (ML) tools to solve complicated reactions.

Feb 2018  
Jan 2013

### **Dhofar University, Sultanate of Oman**

I have worked at Dhofar University of Sultanate Oman as a “Chemical Laboratory Engineer”

#### **Responsibilities & Duties:**

To Conduct Experiments in Chemical Engineering Labs of

- Reactive Process Engineering Lab
  - Fluid Mechanics Lab
  - Fuel Cell Lab
  - Biochemical Engineering Lab
  - Water & wastewater treatment Lab
- Ensure all equipment are maintained, serviced and repaired as required.
  - Diagnose and rectify faults/problems with equipment.
  - Train faculty and students in the use of equipment and techniques.
  - Ensures work is carried out and performed to the required standards.

#### **Undergraduate Research Projects Contribution:**

1. Nutritional study of Omani’s date palm compares to the date palm of Al-Medina.
2. Seawater analysis of Oman region and production of some generic medicine.
3. Study the rate of corrosion on different metal alloys using different seawater.
4. Measurement of pH, heavy metal, vitamin D3, and Microbial Analysis for frankincense.
5. Study the Anti-corrosive properties of frankincense.
6. Modification of Omani Diesel Engine oil using coconut waste.

7. Cellulose–ZnO nanocomposite for medical applications.
8. Modification of Omani Diesel Engine oil using activated carbon and comparison study with well-known engine oil in the market.
9. Comparison study of analysis zam-zam Saudi water with Omani springs water.
10. Synthesis of Zinc Oxide nanoparticles and their antibacterial effect.
11. Production of bio-cellulose facial mask for medical application.
12. Production of bacterial cellulose from cheap resources.
13. Synthesis and Characterization of Iron Oxide Nano-Particles for Magnetic Resonance Imaging (MRI) Contrast Agents.
14. Surface Modified Gd<sub>2</sub>O<sub>3</sub> Nanoparticles For Magnetic Resonance Imaging (MRI) Contrast Agents.

### **Crystalline Chemical Industry Pvt. Ltd, Pakistan**

Dec 2012  
Sep 2012

I have worked at Crystalline Chemicals Industries (Pvt) Ltd as a “Chemical Engineer”

#### **Responsibilities & Duties:**

- Monitoring all equipment’s of biogas & ethanol plant on regular basis for better result.
- To ensure 3M safety and management of man, machinery and materials.
- Data logging of field equipment’s on regular basis.
- Isolation of equipment for maintenance.
- Plant shutdown and startup procedures.
- Monitoring of maintenance jobs; (a) Preventive maintenance (b) Scheduled maintenance
- Performs work activities associated with a Reverse Osmosis Water Treatment Plant.

Jun 2012  
Aug 2011

### **Newage Chemical Industry Pvt. Ltd, Pakistan**

I have worked at Newage Chemicals (Pvt) Ltd as a “Chemical Engineer”

#### **Responsibilities & Duties:**

- Check Machinery & Production Status of the Newage products.
- Check inventory level for daily use and make production, Dispatch & inventory level reports daily.
- Conduct Physical & Chemical tests of raw & produced materials and prepare product quality reports.
- Working for the solution of problems while facing during troubleshooting.
- Conduct safety inspections on-site and report deviations to management.



## **Affiliations**

2012 - present

**Pakistan Engineering Council (PEC)**  
PEC No.: CHEM/09886



## **Languages**

- English – Proficient

- Urdu – Native
- Arabic – Basic
- Korean – Basic

## “ References

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**Name: Dr Seok Ki Kim**

Employer: Ajou University, South Korea

Designation: Assistant Professor (Chemical Engineering Department)

E-mail: seokki@ajou.ac.kr

**Name: Dr Iljeong Heo**

Employer: Korea Research Institute of Chemical Technology (KRICT) and University of Science and Technology (UST), South Korea

Designation: Senior Researcher (KRICT) and Professor (UST)

E-mail: zaiseok@kRICT.re.kr

**Name: Dr Mazhar UI Islam**

Employer: Dhofar University, Oman

Designation: Associate Professor (Chemical Engineering Department)

E-mail: mulislam@du.edu.om