

Ashfeen Ubaid Khan

✉ ashfeenubaid.khan@polimi.it ☎ (+39) 3314017512

📍 Milan, Italy  

EDUCATION AND TRAINING

01/04/2022 – 30/12/2025*

Ph.D (Environmental Engineering)

Milan, Italy

Politecnico di Milano

01/09/2018 – 01/06/2021

M.Sc (Chemistry)

Hangzhou, China

Zhejiang Sci-Tech University

14/08/2014 – 31/07/2017

B.Sc (Honours) (Chemistry)

Aligarh, India

Aligarh Muslim University

EXPERIENCES

1. MARIE CURIE PHD RESEARCHER IN THE EU HORIZON 2020 REMEDI PROJECT

Project Website: <https://warwick.ac.uk/fac/sci/eng/remedi/>

Academic Supervisor: Prof. Alberto Guadagnini

Industrial Supervisor: Dr. Patrick Jacobs

Politecnico di Milano (Academic Host) | **Milan, Italy** | 04/2022 – Present

- Investigated the transport and removal of contaminants (pharmaceutical) by studying their interaction with natural and engineered colloids (e.g., surfactant modified-Montmorillonite clays, Fe_3O_4 nanoparticles) in batch and fixed-bed column scale.
- Developed and applied reactive tailored transport models (MATLAB, Python) to simulate contaminant behavior in porous media, incorporating Bayesian model selection and optimization and global sensitivity analysis.
- Molecular scale modeling using Molecular dynamics dynamics and DFT methods for adsorption of contrast media agents on various substrates.

Lario Reti Holding Spa (Research Secondment) | **Lecco, Italy** | 10/2024 – Present

- Developed an innovative water quality index model incorporating novel global sensitivity analysis to enhance water distribution monitoring.
- Performed accredited water quality analyses (UNI EN ISO, APAT CNR) on drinking and wastewater, quantifying microbial indicators (*Escherichia coli*, *Enterococcus* spp., coliforms, etc.), ions (IC), and metals (ICP-OES) within an ISO/IEC 17025 framework.

TAUW GmbH (Industrial Host) | **Berlin, Germany** | 05/2023 – 04/2024

- Involved in PFAS site investigations at industrial locations, including Audi Ingolstadt facility, managing sampling and data analysis.
- Executed site assessments in compliance with German environmental regulations.

2. RESEARCH ASSISTANT

Zhejiang Sci-Tech University | **Hangzhou, China** | 09/2018 – 06/2021

Supervisor: Dr. Lingxiangyu Li

- Developed analytical methods for the transformation, selective speciation and quantification of transformed nanoparticles (e.g., Ag_2S) in complex environmental matrices, human bio-fluids, soil and sediment.
- Analyzed nanoparticle stability, dissolution kinetics, and biotic interactions (bio-corona formation) in simulated fluids to understand their transport, toxicity to *Escherichia coli*, and fate.

PUBLICATIONS

- Fate and risk of metal sulfide nanoparticles in the environment

(Equal Contribution from **Ashfeen Ubaid Khan** and Zhang Xiaoxia)

Ashfeen Ubaid Khan, Zhang, X., Sharma, V.K. and Lingxiangyu Li. *Environmental Chemistry Letters* 18, 97–111 (2020). DOI: [10.1007/s10311-019-00920-x](https://doi.org/10.1007/s10311-019-00920-x)

- Transformations of Ag_2S nanoparticles in simulated human gastrointestinal tract: Impacts of the degree and origin of sulfidation

(Lead author)

Ashfeen Ubaid Khan, Zhenlan Xu, Xiaoting Qian, Aimee Hong, Qing Tang, Tao Zeng, Melanie Kah, Lingxiangyu Li. *Journal of Hazardous Materials*, Volume 401, 123406 (2021).

DOI: [10.1016/j.jhazmat.2020.123406](https://doi.org/10.1016/j.jhazmat.2020.123406)

- Identification and Speciation of Nanoscale Silver in Complex Solid Matrices by Sequential Extraction Coupled with Inductively Coupled Plasma Optical Emission Spectrometry
(Co-authored : contributed to sequential extraction method development)

Aimee Hong, Qing Tang, **Ashfeen Ubaid Khan**, Zhenlan Xu, Xinyu Bian, Haijin Lou, Fei Dang, Yawei Wang, Dahui Lin, Juliane Filser and Lingxiangyu Li. *Analytical Chemistry ACS*, 93, 4, 1962-1968 (2021). DOI: [10.1021/acs.analchem.0c04741](https://doi.org/10.1021/acs.analchem.0c04741)

- Emerging investigator series: chemical transformation of silver and zinc oxide nanoparticles in simulated human tear fluids: influence of biocoronae

(Equal Contribution from Lingxiangyu Li and **Ashfeen Ubaid Khan**)

Lingxiangyu Li, **Ashfeen Ubaid Khan**, Xiang Z, Xiaoting Q, and Yawei Wanga (2021). *Environmental Science: Nano*, 8(9), 2430-2440. DOI: [10.1039/D1EN00566A](https://doi.org/10.1039/D1EN00566A)

- In-silico mechanistic analysis of adsorption of Iodinated Contrast Media agents on graphene surface.

(Lead Author)

Ashfeen Ubaid Khan, Giovanni Porta, Monica Riva, Alberto Guadagnini (2024). *Ecotoxicology and Environmental Safety*, 280, 116506. DOI: [10.1016/j.ecoenv.2024.116506](https://doi.org/10.1016/j.ecoenv.2024.116506)

PUBLICATIONS (in Press)

- A Unified Framework for Assessing Water Quality Indices under Data and Model Weight Uncertainty

(Lead Author)

Ashfeen Ubaid Khan, Giovanni Porta, Monica Riva, Raffaele Rossi Ronca, and Alberto Guadagnini*. Submitted (Under review in *Journal Water Research*).

- Multiscale Investigation of Iohexol and Diatrizoic Acid Removal Using Modified Montmorillonite Organo-Clay: Integrating Experimental and Numerical Upscaling Studies

(Lead Author)

Ashfeen Ubaid Khan, Giovanni Porta, Monica Riva, and Alberto Guadagnini. (Submitted to *ACS ES&T Engineering*).

CONFERENCES AND SEMINARS

EGU General Assembly 2025

Vienna

Oral presentation

27/04/2025 – 02/05/2025

Title: *Removal of Iodinated Contrast Media Using Surfactant-Modified Montmorillonite Clay: Batch and Column Studies.*

EGU General Assembly 2024

Vienna

Poster presentation

14/04/2024 – 19/04/2024

Title: *Mechanistic study of the adsorption of Iodinated Contrast Media agents on monolayer Graphene surface in-silico.*

Goldschmidt 2023

Lyon

Poster presentation

09/07/2023 – 14/07/2023

Title: *Chemical speciation and microbial growth of natural spring waters associated with diverse hydrogeological settings in the area of Lecco (Italy).*

14th TAUW Soil Seminar 2023

Milan

Oral presentation

14/06/2023 – 15/06/2023

Title: *Removal of Iodinated Contrast Media agents using modified geomaterials.*

Interpore 2023

Edinburgh

Poster presentation

22/05/2023 – 25/05/2023

Title: Mechanistic studies on the adsorption of Iodinated Contrast Media agents on monolayer graphene in-silico.

CPJRC Seminar

Remote sensing technology applications.

Beijing

19/10/2021 – 22/10/2021

INVITED TALKS AND LECTURES

TAUW Soil Webinar on Data Analysis | Online | 10/2024

- Led a technical webinar for TAUW employees and water sector professionals, focusing on innovative tools for water quality characterization.

International Festival of Engineering | Milan, Italy | 09/2024

- Represented REMEDI ITN: Conducted interactive presentations for diverse audiences, from young students to industry professionals.

E-Learning Module on Emerging Contaminants | Online | 2024

- Developed and presented a comprehensive chapter for an online course focusing on remediation emerging contaminants using Iron geomaterials (as part of REMEDI project dissemination).

DIGITAL SKILLS

Computational Chemistry & Molecular Modeling: GROMACS (Molecular Dynamics), QUANTUM ESPRESSO (DFT), BIOVIA Materials Studio (DFT), QSAR, etc

Numerical modeling/Analysis & Visualization: Experience in : **MATLAB** (transport and adsorption Simulation using PDEs), **Python** (sensitivity analysis and monte carlo), and **R** (compositional data), GraphPad Prism, Edraw-Max, etc

Other: QGIS, ImageJ, Geochemists Workbench and PHREEQC, MS Office, Overleaf, etc

LAB SKILLS

Spectrometry & Chromatography: ICP-OES & AAS (*trace metal analysis*), UV-Vis & HPLC (*quantitative analysis*), Ion Chromatography (*dissolved ion quantification*), FT-IR (*surface analysis*)

Material & Nanoparticle Characterization: HR-TEM / SEM-EDS (*morphological & elemental analysis*), XRD (*phase identification*), DLS (*particle size & zeta potential*)

Water Quality & Microbiological Analysis: Standard Methods for Water Testing (pH, conductivity, TSS by Gravimetry, BOD, COD), Microbiological Culturing (plate count, MPN for *Escherichia coli*, coliforms, *Enterococcus* spp.) according to ISO standards.

HONOURS AND AWARDS

JK Prime Ministers Special Scholarship

01/08/2014

All India Council for Technical Education — Full funding during Bachelor's degree programme at AMU.

President Scholarship

14/09/2018

Zhejiang Sci-Tech University — Full funding during Master's degree programme at ZSTU.

Young Talents Scholarship (ANSO)

01/08/2021

Institute of Chemistry, Chinese Academy of Sciences — Awarded by Alliance of International Science Organisations.

OTHER INFORMATION

Languages: Kashmiri (Mother tongue), English - Fluent (Oral/Written) (IELTS 7)

Interests: Cricket, Swimming, Himalayan Wildlife

REFERENCES

Prof. Alberto Guadagnini, Professor
Politecnico di Milano, Italy
✉ alberto.guadagnini@polimi.it | ☎ (+39) 0223996263
Website: <https://www.mipore.polimi.it>

Prof. Monica Riva, Professor
Politecnico di Milano, Italy
✉ monica.riva@polimi.it | ☎ 02-23996214
Dr. Patrick Jacobs, Technical Director
TAUW GmbH, Germany
✉ patrick.jacobs@tauw.com | ☎ (+49) 15209395641

Dr. Lingxiangyu Li, Associate Professor
Hangzhou Institute of Advanced Studies, University of Chinese Academy of Science, China
✉ lingxiangyu.li@ucas.ac.cn