Mohammad Monir

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EDUCATION

PhD Student, IFP Energies Nouvelles (IFPEN) & Sorbonne University, Paris, France, November 2025 – Present

- Project title: Mesoscopic modelling of PFAS aggregation and adsorption on model mineral surfaces
- Use coarse-grained and dissipative particle dynamics approaches to investigate PFAS–surface interactions, surfactant self-assembly, electrolyte effects, and adsorption mechanisms at mineral–water interfaces.
- Analyse the influence of PFAS different properties on adsorption performance and interfacial behaviour.

Erasmus Mundus Master of Theoretical Chemistry and Computational Modelling (EMTCCM), KU Leuven, Belgium, September 2022 – July 2024

- Fully Funded Scholarship from Erasmus Mundus.
- Main courses are namely quantum chemistry, Density Functional Theory, Solid State Physics, Advanced Computational Techniques, Theoretical Methods for Simulation of Materials, and Multiscale, Machine Learning and QSAR Methods Applied to Biomolecules.
- Graduated with Cum laude.

Bachelor of Chemistry with Minors in Economics and Arab and Islamic Civilizations, The American University in Cairo (AUC), Egypt, September 2018 - January 2022

- Fully Funded Scholarship from USAID December 2017 – January 2022.
- Main courses are namely organic, biochemistry, inorganic, physical, polymer, and analytical chemistry.
- Highest Honours (Summa Cum Laude) with a cumulative GPA of 3.83 and major GPA of 3.95.

EXPERIENCE

Research Assistant, Vrije Universiteit Brussel, (ALGC: “General Chemistry Group”), Chemistry Department. October 2024 – October 2025

- Conduct literature reviews and analyse thermochemical and electrochemical data for advanced energy storage materials using both experimental and theoretical approaches.
- Utilize Matlantis and machine learning interatomic potentials to perform molecular dynamics simulations for predicting thermochemical behaviour of energy storage materials.

Research Internship, Donostia International Physics Centre, San Sebastian, August 2024 – October 2024

- Internship project title: Magnetic anisotropy of organic radicals (m-xylene based polyradicals).
- Performing d Density Functional Theory (DFT) calculations to optimize molecular geometries and calculate Zero-Field Splitting (ZFS) parameters for m-xylylene based polyradicals, while cross-validating results using Multiconfigurational Self-Consistent Field (MCSCF) methods.

Master Research Internship, Research institute in Molecular Chemistry, University of Nantes, January 2024 – June 2024

- Internship project title: Complexation properties of the cationic form Ra^{2+} with various model chelators.
- Performed 2c-DFT calculations of different metal exchange and ligand exchanges reactions in gas phase and using the solvation model of SMD which is followed by using Hess cycle to do some free energy calculations.

Research Internship, Chemistry Department, KU Leuven, February 2023 – May 2023

- Internship project title: Reactivity of indene and cyano-indene with ions in space such as helium.
- Performed quantum chemistry calculations (CCSD(T) and DFT) of the long-range potential of these reactions and computed new rate coefficients using a modified capture theory.

Teaching Assistant, Chemistry Department, The American University in Cairo, August 2021 – June 2022

- Courses are thermodynamics, organic chemistry II, analytical chemistry II and its lab, physical chemistry III, and Egypt water crisis: challenges and solutions.
- Conducted revision, review, and problem sessions for the students and support them in carrying out their experimental work.

Bachelor Research Project, Chemistry Department, The American University in Cairo, January 2021 – October 2021

- Project title: Use of green technology based on Novel Functionalized biodegradable polymeric resins for the removal of toxic heavy metals from wastewater.
- Investigated chitosan-based adsorbents for removing heavy metals from wastewater and optimizing conditions for maximum efficiency through crosslinking.

AWARDS

The Jehane Ragai and John Thomas Highest Achiever in Chemistry Award, The American University in Cairo, January 2022

- The award is given to the student having the highest GPA in Chemistry at the undergraduate level.

Silver Medal, International Genetically Engineered Machine Competition, virtual, November 2020

- Used synthetic biology to create a designed circuit to control the expression of the hybrid transcriptional activator of COVID-19.

PUBLICATIONS

Research Paper, MDPI Polymers Journal, 2024

- Talked about novel high-performance functionalized and grafted bio-based chitosan adsorbents for the efficient and selective removal of toxic heavy metals from contaminated water in a twenty-paper research.

SKILLS

Languages: Native in Spoken and written Arabic, Fluent in Spoken and written English, Intermediate in Dutch, and Beginner in French and German.

Computer and Quantum chemistry: Proficient user of Office Suite (Word, PowerPoint, Excel) and Quantum chemistry programs such as (Molpro, Avogadro, Gaussian, Dirac, Molden, Orca, and VASP) in Linux environment, Proficient user of Python, C+, Fortran programming languages and machine learning software of Matlantis.