Moyassar Meshhal

PhD student and research assistant at the universty of Rostock.

Address (work): Albert Einstein Straße 23-24, 18059 Rostock, Germany.
Email (work): moyassar.meshhal@uni-rostock.de
Email (personal): moyassar.meshhal@gmail.com

Research interests

Computational Chemistry/Physics, 2D Materials, MD Simulations, Machine learning

Education

Oct. 2019 – Present	**University of Rostock** – Rostock, Germany PhD in Physics **Project:** 2D Materials Simulations. **Mentor**: Prof. Dr. Oliver Kühn.
Sep. 2016 – Feb. 2019	**Menofia University** – Menofia, Egypt MSc in Computational Chemistry **Thesis Title:** "A Computational Study on the Structure and Stability of Different Tautomers of Phenanthroline Analogues" **Mentors**: Prof. Dr. Ahmed El-Nahas & Dr. Mohamed Shibl.

Publications

2022 **The Role of Hydrogen-Bonded Bridges for the Diffusion of Water Confined Between Graphene Oxide Layers**
Moyassar M. Meshhal, Oliver Kühn.
submitted. ChemRxiv Link

2019 **A Thermochemical Computational Study on Hydroxyquinlines and their Azulene Analogues**
Moyassar M. Meshhal, Safinaz H. El-Demerdash, Ahmed M. El-Nahas.
Journal of Molecular Structure, 1183 (2019) 70-77.

2018 **A Computational Study on Molecular Structure and Stability of Tautomers of Dipyrrole-Based Phenanthroline Analogue**
Moyassar M. Meshhal, Mohamed F. Shibl, Safinaz H. El-Demerdash, Ahmed M. El-Nahas.
Computational and Theoretical Chemistr, 1145 (2018) 6–14.

Professional memberships

2019 – Present	**Egypt's delegate** for: International Younger Chemists Network (**IYCN**)
	Description: *An affiliated organization of the International Union of Pure and Applied Chemistry (IUPAC), connecting chemists in the early stages of their career.*

Technical skills

Programming languages

Familiar with: Python, Bash scripting

Software

Linux, Vim, LaTeX, Git, Anaconda, Jupyter-Notebook

Cmputational chemistry packages

Gaussian, Orca, CP2K, DFTB+, CP-PAW

Languages

Arabic (Mother tongue), **English** (advanced), **German** (beginner)

Other interests

Reading, cycling.