RAFAIL **LINGAS**

Email: **rafaling@iti.gr**

WORK EXPERIENCE

10/2025 – CURRENT

Postdoctoral Researcher, Centre for Research & Technology (CERTH), Greece

Project Management, Quantum Computing.

- Design and development of a comprehensive Quantum Computing Course (educational material, curriculum, and programming exercises).
- Exploring and prototyping Python-based pipelines for quantum computing applications.
- Participation in research projects involving technical contributions, project meetings, and collaboration on project deliverables.

03/2024 – 09/2025

Principal Research Engineer, Linköping University, Sweden

Computational research in Photochemistry using quantum methods.

- Combining quantum chemical methods with molecular dynamics.
- Developed Python-based tools to streamline and scale simulation workflows.
- Supervising PhD students, providing direction on research objectives.

09/2024 – CURRENT

Data Scientist, eSpyros Data Solutions, Remote

Project-based engagements in advanced data science solutions.

- Built and deployed forecasting models and machine learning solutions to drive analytics, reporting, and business insights.
- Developed and maintained robust data pipelines for processing large datasets using Python.

09/2020 – 03/2022

Researcher in Chemistry, Aristotle University of Thessaloniki, Greece

Computational Study of Mechanical and Electronic Properties of Pillared Graphene Structures, Design and Screening of Pillared Structures, Flexible Device Fabrication and Measurements.

- Automating workflow using Python. High-Performance Computing.
- Worked extensively with many computational quantum chemistry programs.

10/2018 – 12/2019

Supply Teacher, Randstad Education, Cambridge, United Kingdom

- Teaching mathematics and computer science to secondary schools.

Summer of 2017,2018, and 2019

English Teacher, British Study Centres, Oxford, United Kingdom

- Teaching English to young students from all around the world.

EDUCATION

07/2020 – 12/2023

PhD in Computational Quantum Chemistry, Aristotle University of Thessaloniki

Software Development and Application for the analysis and visualization of the induced magnetic field for the theoretical study of aromaticity of organic and inorganic molecular systems.

- Designed and implemented a cross-platform scientific software tool in Python for quantum chemical calculations, analysis, and visualization.
- Managed large datasets and complex quantum mechanical simulations on HPC clusters, optimizing for performance and storage.
- Sole developer of a custom scientific software suite used in multiple peer-reviewed publications; actively supported its adoption by students in their thesis projects.

10/2017 – 06/2020

Master's Degree in Computational Quantum Chemistry, Aristotle University of Thessaloniki

Analysis of the induced magnetic field in natural localized orbital contributions. 9.5

- Developed Python tools for parsing and processing complex simulation output data.
- Building data pipelines for analyzing magnetic field contributions in molecular systems.

2011 – 2017

Bachelor's Degree in Physics, Aristotle University of Thessaloniki

4th year- Specialization in programming (thesis). EQF level 6

SKILLS

- **Programming & Data Science:** Expert in Python, predictive modeling, and data analysis. Proficient in Bash; working knowledge of C++ and JavaScript**.**
- **Scientific Software Development**: Developed GUIs, created 3D visualizations for data analysis and simulation results.
- **Publication Track Record**: Proven capability to produce high-quality scientific output under peer review.
- **Cross-disciplinary collaboration**: Bridging chemistry, physics, and computer science to translate complex problems into computational solutions.

PUBLICATIONS

- Lingas, R., Charistos, N. D., & Muñoz-Castro, A. (2024). Borospherene in the Nanohoop. *Chem. Eur. J,* DOI: 10.1002/chem.202402027
- Lingas, R., Charistos, N. D., & Muñoz-Castro, A. (2023). Charge Delocalization and Aromaticity of Doubly Charged Double-walled Carbon Nanohoops. *Phys. Chem. Chem. Phys,* DOI: 10.1039/D3CP01994B
- Lingas, R., Muñoz-Castro, A. (2023). Local and Global Aromaticity under Rotation. Analysis of Two- and Three-Dimensional Carbon Nanostructures. *Phys. Chem. Chem. Phys,* DOI: 10.1039/D3CP00569K
- Lingas, R., Charistos, N. D., & Muñoz-Castro, A. (2021). Aromaticity of ortho and meta 8-Cycloparaphenylene and their dications: Induced Magnetic Field Analysis with Localized and Delocalized Orbitals in Strained Nanohoops. ChemPhysChem, DOI: 10.1002/cphc.202100057

All publications were based on research done using my own software built with Python.