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GitHub Profile

LinkedIn Profile

EDUCATION

•**Computational Chemistry PhD** *2024-2028*

The University of Manchester, Manchester, UK

•**Master of Chemistry (MChem)** *2021-24*

Newcastle University, Newcastle-upon-Tyne, UK First Class

EXPERIENCE

•**Academic Researcher in Computational Chemistry** *September 2024 - Present*

The University of Manchester

- Lead developer on the WebAQME and AQMEasy projects to automate computational chemistry tasks via a web app (Flask) and a desktop app (PySide6), respectively.
- Collaborated on chemical reactivity projects with two different experimental groups (organic and inorganic materials).
- Tech stack: Python (PySide6, Flask, SQLAlchemy, RDKit), HTML5, CSS, JavaScript

•**Research Internship in Computational Chemistry** *June 2023 - September 2023*

Newcastle University

- Worked on a machine learning project which looked at using an LSTM model to predict spectroscopic lineshapes from molecular geometry data. The project was presented at two conferences (local via poster and national via talk), and the results were published in a review paper.
- Learned Linux & bash scripting, and developed a good understanding of machine learning and data science fundamentals.

PERSONAL PROJECTS

•**Writing Tracker + Pomodor*ish* Timer (Qt Framework Practice)** *2024*

Desktop apps to track a writing goal with approximate required words per day, and a focus timer for productivity.

- Packaged with PyInstaller. Available on GitHub (hyperlinks): Tracker and Timer.
- Technology Used : Python3, PySide6/PyQt6, PyInstaller.

TECHNICAL SKILLS AND INTERESTS

Languages: Python, Bash, JavaScript, C
Libraries: Pandas, NumPy, RDKit
Developer Tools: Git, GitHub, VSCode, Vim
Systems: Linux, HPC/cluster computing
Web Dev: Flask, HTML5, CSS
Databases: SQLAlchemy
Areas of Interest: Low-level programming, app development

POSITIONS OF RESPONSIBILITY

•**Theoretical Chemistry Group Committee Member** Royal Society of Chemistry *December 2024 - Current*

- Appointed via election open to the entire group, which includes academics and people in industry primarily but not exclusively based in the UK .
- Organised an online scientific conference with over 150 registered attendees, 10 contributed talks, 60 contributed posters and two major plenary speakers.

•**Supervisor for a Summer Student** Trujillo Research Group *June 2025 - August 2025*

- Designed a project for a second year chemistry undergraduate. The project can be found on GitHub.
- Mentored and supervised the student for 6 weeks.