Julia Kaczmarek

Developer & Researcher
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GitHub (jak713) | Linkedin (yuliakaczmarek)

Skills

Programming Languages:	Python, Bash, HTML, CSS, JavaScript
Libraries/Frameworks:	PySide6, Pandas
Software Development:	Desktop Application Development, Object-Oriented Programming, MVC Architecture, Version Control
Tools / Platforms:	Linux, Git, GitHub, LaTeX, HPC
Databases:	SQL

Education

The University of Manchester — Manchester, UK
Computational Chemistry PhD (Doctor of Philosophy) — September 2024 - February 2028 (Expected)

Newcastle University — Newcastle-upon-Tyne, UK
Chemistry MChem (Master of Chemistry) — September 2021 - July 2024
Percentage: 75.7%

Experience

The University of Manchester | Academic Researcher Manchester, UK | September 2024 - Present

- Leading development of AQMEasy (PySide6), delivering an application that automates computational chemistry workflows and reduces technical barriers for researchers. This requires a consistently high level of initiative, resilience and problem solving.
- Provided computational chemistry expertise to support experimental reactivity projects across organic and inorganic materials groups. Bridged computational predictions with experimental validation across multiple collaborations requiring high organisation, time management, teamwork and communication skills.
- Presented research at international conferences, translating complex technical findings for diverse audiences and strengthening networking skills.
- Supervised summer student in developing an automation interface for quantum chemistry input files, delivering a functional tool. Continued to mentor the student since by checking in monthly on university and career progress.

The University of Manchester | Graduate Teaching Assistant Manchester, UK | January 2025 - Present

- Supervised weekly computational lab sessions of 20-30 students, teaching Gaussian software and providing technical guidance for computational chemistry calculations.

Newcastle University | Research Intern Newcastle-upon-Tyne, UK | June 2023 - September 2023

- Optimised an LSTM model to predict spectroscopic line-shapes from molecular geometry, achieving an improved accuracy over existing methods of 96%(2% increase). Presented work at local (poster) and national (talk) conferences, with results published in a review paper. Gained proficiency in Linux, bash scripting, and machine learning fundamentals.

Projects / Open-Source

AQMEasy | Link *Python, Qt*

- Developing a modular desktop GUI for the AQME computational chemistry software, designed to make quantum chemistry calculations accessible to researchers with limited programming experience.
- Automates workflow setup, job submission, and results analysis for common computational chemistry tasks, reducing setup time and technical barriers.

QTAIM Visualiser | Link *Python, py3dmol*

- Developed a Jupyter Notebook tool for visualising non-covalent interactions from QTAIM analysis performed with Multiwfn software.

- Automates atom assignment between interactions and enables parameter-based searching, streamlining analysis of molecular interactions.

NBO Visualiser | Link *Python, py3dmol*
- Developed a Jupyter Notebook tool for visualising Natural Bond Orbital (NBO) analysis results from ORCA+NBO7 calculations, including SOPT and NPA data.
- Interfaces with QTAIM Visualiser to compare and validate non-covalent interaction predictions across different analysis methods, saving multiple hours of work.

twordle (Terminal Wordle) | Link *Python, curses*
- Developed a terminal-based implementation of the popular word game Wordle using the curses library for an interactive CLI interface.

Certifications

- Introduction to JavaScript- **CodeFirstGirls 2025**
- Introduction to C#- **CodeFirstGirls 2024**
- Introduction to Data and SQL (Highly Commended Candidate) - **CodeFirstGirls 2023**
- Introduction to Python and Apps - **CodeFirstGirls 2023**

Honours & Awards

- 2024 Neil Hughes Prize at Newcastle University for contributions to the school
- 2023 Levin Prize at Newcastle University for meritorious performance in Stage 3
- 2022 SCI Prize at Newcastle University for meritorious performance in Stage 2

Casual/Part-time Work Experience

Developed strong problem-solving, communication, and attention to detail through 6+ years in customer-facing and operational roles, with experience working under pressure, adapting to varied requirements, and maintaining high standards in fast-paced environments.

- Team Member at Everyman Cinema (December 2023 - November 2024)
- Team Member at Newcastle University Students' Union (September 2023 - September 2024)
- Kitchen Assistant at J D Wetherspoon (February 2020 - September 2023)
- Retail Assistant at Primark (January 2018 - February 2020)

Volunteering & Other Interests

Royal Society of Chemistry Theoretical Chemistry Group | Committee Member January 2025 - Present
- Organised an online scientific conference with over 150 registered attendees, 10 contributed talks, 60 contributed posters and two major plenary speakers.
- Appointed via election open to the entire group, which includes academics and people in industry primarily but not exclusively based in the UK.

Chemistry Department (Newcastle University) | Chair of Student-Staff Committee September 2023 - June 2024
- Chaired frequent meetings between student representatives and academic staff, setting agendas and facilitating discussions on course content, assessment, and student welfare.
- Gathered feedback from chemistry students, raising concerns about course layouts and access, and advocating for improved course delivery.

Figure Skating Society (Newcastle University) | Secretary September 2022 - July 2023
- Provided minutes for all committee meetings and managed communications to members.
- Organised an end-of-year ball with two other societies for an overall turnout of 100+ people.

My interests include collecting sea glass and interesting rocks on beaches, tabletop gaming, handmade cards for people, painting, playing guitar, playing Minecraft with friends, and learning things that interest me. Started the OSSU CS curriculum because I am interested in the underlying theory of computer science.