

Frazer N. Forrester

Computational Materials Scientist | MEng (Hons) | AFHEA | AMIChemE

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Profile

PhD researcher in Chemistry with a Master's in Chemical Engineering, currently specialising in computational modelling of energy materials, with a focus on solid-state batteries. Experienced in applying classical and quantum mechanical methods to study defects, disorder, and dynamics in complex systems. Skilled in Python, Bash, workflow automation, and high-performance computing, with a strong record of collaboration, supervision, and communication. Motivated to apply scientific rigour and problem-solving to engineering, energy, and technology challenges.

Technical Skills & Expertise

- **Computational Methods & Tools:** Density Functional Theory (DFT), Molecular Dynamics (classical and *ab initio*), and Nudged Elastic Band (NEB), Machine Learning Interatomic Potentials (MLIPs); simulation packages including VASP, LAMMPS, GULP, CHGNet; visualisation with VESTA, Ovito.
- **Workflow Automation & HPC:** High-performance computing on Tier 1–3 systems; Linux/Unix environment; job scheduling with Slurm and PBS
- **Programming & Scripting:** Python (pymatgen, ASE, NumPy, Matplotlib, Pandas), Bash, Git, \LaTeX .
- **Data Analysis & Communication:** Handling large datasets, working with structured/unstructured formats, building reproducible workflows, and producing technical reports, publications, and visualisations.

Professional & Transferable Skills

Collaboration • Communication • Problem-Solving • Research & Project Management • Supervision & Mentoring • Leadership • Adaptability • Initiative • Critical Thinking • Attention to Detail • Time Management • Funding Acquisition

Experience

PhD Researcher, Newcastle University, UK Sept 2020 – Present

- Developed expertise in classical and *ab initio* methods for solid-state materials modelling, using tools such as GULP, LAMMPS, and VASP.
- Built a collaborative research group from its inception to 20+ members, chairing weekly tutorials and meetings.
- Collaborated nationally and internationally with researchers on multidisciplinary projects.
- Supervised and trained MChem and PhD students, producing publication-quality research.
- Secured >200,000 CU (40k equivalent) through successful HPC grant applications via EPSRC's Materials Chemistry Consortium (MCC), on Archer 2.
- Published peer-reviewed publications and presented work at national and international conferences.
- Active affiliate of the EPSRC CDT in Renewable Energy Northeast Universities (ReNU).
- Served on the organising committee for the School of Natural and Environmental Sciences Research Symposium.
- Member of CCP5 (Collaborative Computational Project for the Study of Condensed Phase Systems).

Research Assistant in Inorganic Materials, Newcastle University, UK Nov 2023 – Nov 2024

Focus: Modelling defects, disorder and bulk properties of solid-state energy materials using DFT, MD/AIMD and, more recently, Machine Learning Interatomic Potentials (MLIPs).

- Trained and supervised several PhD and MChem students; received 5 nominations for Newcastle University's 'The Education Awards (TEAs) 2024'.
- Contributed to peer-reviewed publications.

- Member of the Research Associate Committee, contributing perspectives and actions on research, education, management, and EDI at school-level.
- Active in the *Python in Chemistry* group, advocating for the integration of computational tools and programming in chemistry education and research.

Lead Demonstrator, Newcastle University, UK

Dec 2023 – Feb 2024

- Modernised the *Scientific Computing for Chemists* module, improving student engagement and aligning content with current chemistry research trends.
- Demonstrated diverse problem-solving methods, emphasising multiple “correct” approaches to foster critical thinking and adaptability.

Graduate Teaching Assistant, Newcastle University, UK

Sept 2021 – Nov 2023

Overview: Taught and demonstrated both laboratory and computational methods across stages: Stage 1 – Scientific Computing for Chemists, General Chemistry; Stage 2 – Physical Chemistry; Stage 3 – Advanced Practical Physical Chemistry.

- Delivered introductory Python lessons with applications in scientific computing and data analysis.
- Instructed on various characterisation and synthesis techniques (e.g. UV-Vis, Fluorescence, etc.).
- Debugged experimental setups, marked and moderated student work, and provided formative and substantive feedback to support student development.
- Built strong interpersonal relationships with students, academics, and technical staff, fostering a supportive and collaborative learning environment.

Exam Invigilator, Newcastle University, UK

May 2022 – August 2022

Maintained exam integrity through vigilant time-keeping and strict protocol adherence.

Education

Doctor of Philosophy (PhD) in Chemistry, Newcastle University

Sept 2020 – Dec 2024

Thesis: “Theoretical Insights into Defects and Dynamics in Solid Electrolyte Materials”

Overview: Utilised classical and quantum mechanical computational techniques to expedite the discovery and optimisation of fast-ion conducting electrolytes for safe and energy-dense solid-state batteries.

Masters of Chemical Engineering (MEng (Hons)), Lancaster University

Sept 2016 – Jun 2020

Modules: Mass and Heat Transfer, Engineering Analysis, Particle Technology and Separation Processes, Thermodynamics, Leadership in Technology, Advanced Process Transfers, Energy Conversion, Design and Process Safety, Nuclear Fuels and Energy Conversion, Electrochemical Engineering, among others.

- Gained proficiency in key engineering software and techniques, including HAZID, HAZOP, P&ID, PFD, Aspen, Ansys, and CAD, applied extensively throughout my studies.

Dissertation: “Isotopic Lithium Diffusion in Stoichiometric Solid-State Systems for Lithium Separation”

Overview: Utilised classical mechanical simulation techniques to assess a potential lithium-isotope enrichment technology proposed as an enabler for nuclear fusion commercialisation.

- Developed advanced computational modelling skills, particularly in Molecular Dynamics (MD) simulations using HPC, which contributed to securing a PhD studentship.
- Demonstrated resilience and adaptability by successfully completing a research project beyond the formal scope of the degree curriculum.

Third-Year Design Project: “Production of Next Generation Ammonia through Direct Electrochemical Synthesis”

- Collaborated on route selection and produced a comprehensive design report for a plant capable of producing 1,000 tonnes/day of next-generation ammonia.
- Independently designed a multi-faceted water purification system centred on reverse osmosis.
- Applied hazard mitigation and prevention techniques (e.g. HAZID, HAZOP) and implemented key design elements, such as P&IDs.

Professional Memberships

- Associate Fellow of the Higher Education Academy (AFHEA).
- Associate Member of The Institute of Chemical Engineering (AMIChemE).
- Affiliate Member of the Royal Society of Chemistry.

Awards & Funding Acquired

- Awarded the Millennium Volunteers 100- and 200-hour certification, along with the Sport Award (MV50), by Gerry Frobisher MBE on behalf of the Welsh Government for services to the local area.
- Achieved IChemE/RSC-accredited JMP 'Design of Experiments' certification.
- Received a Faraday Institution Conference Bursary (1 of 20 recipients) (Sept. 2023).
- Secured Newcastle University Doctoral College Enhancement Fund (£2,000) to visit the groups of Profs. David O. Scanlon (University College London) and Aron Walsh (Imperial College London) (Feb. 2023).
- Awarded Newcastle University School of Natural and Environmental Sciences Travel Award (£600) (May 2022).

Additional Experience

Diagnostic Drain Cleaner and Repair Worker , Drain Medic	2016 - 2020
Commercial Window Cleaner , Window Cleaner.Co	2016 - 2020
Bartender and Hospitality , Greene King	2014 - 2016