Frazer N. Forrester

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

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Profile

Driven computational materials scientist specialising in atomistic modelling—both quantum and classical—leveraging high-performance computing to investigate defects and dynamics in solid-state systems and optimise materials for energy applications. Currently a Research Assistant at Newcastle University, I am experienced in collaboration, supervision, and multidisciplinary research, committed to advancing impactful work at the intersection of energy, environment, and engineering.

Technical Skills & Expertise

- **Computational Methods:** Density Functional Theory (DFT), Classical Molecular Dynamics (MD), *Ab initio* Molecular Dynamics (AIMD), Nudged Elastic Band (NEB).
- **High-Performance Computing (HPC):** Experience with Tier 1–3 systems, proficient in Slurm and PBS schedulers.
- **Programming & Scripting:** Python (e.g. `pymatgen`, `ASE`, `NumPy`, `Matplotlib`, `Pandas`), Shell scripting (Bash, Zsh), LaTeX.
- **Visualization Tools:** Atomic visualization software (Ovito, VESTA)
- **Data Analysis & Visualization:** Expertise in extracting insights and creating high-quality visuals for technical reports.

Soft Skills

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

Experience

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

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 projects, resulting in 5 anonymous nominations for Newcastle University's 'The Education Awards (TEAs) 2024'.
- Research Associate (RA) Committee Member—advocating for RA interests and providing perspectives on research, education, management, and Equality, Diversity, and Inclusion (EDI) at school-level committees.
- Active contributor to the 'Python in Chemistry' group—advocating for the integration of computational tools and programming in chemistry education and research.

PhD Researcher, Newcastle University, UK — Sept 2020 – Present

- Developed expertise in classical and *ab initio* methods for solid-state materials modeling, using tools such as `GULP`, `LAMMPS`, and `VASP`.
- Established and cultivated a collaborative research and lab culture, growing the group from its inception to over 20 members.
- Chaired weekly group meetings and tutorials to foster collaboration and skill development among members.
- Built relationships and collaborated with national and international researchers on multidisciplinary projects.
- Supervised MChem and PhD students, producing research of publication-ready quality.
- Prepared successful applications for HPC resources through the EPSRC's Materials Chemistry Consortium (MCC) on Archer 2, securing over 200,000 CUs (£40,000 equivalent) for personal and group research projects.
- Presented research at national and international conferences, engaging diverse academic and professional

audiences.

- Active affiliate of the EPSRC Centre for Doctoral Training in Renewable Energy Northeast Universities (ReNU).
- Served on the organising committee for the School of Natural and Environmental Sciences Research Symposium, contributing to event planning and execution.
- Active member of CCP5 (Collaborative Computational Project for the Study of Condensed Phase Systems), engaging in workshops and discussions.

Lead Demonstrator, Newcastle University, UK Dec 2023 – Feb 2023

- Modernised the 'Scientific Computing for Chemists' module with up-to-date techniques and tools, 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 in scientific computing.

Graduate Teaching Assistant, Newcastle University, UK Sept 2021 – Nov 2023

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

- Delivered introductory Python programming lessons with a focus on practical applications in scientific computing and data analysis.
- Instructed on various characterization 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

Selected as a paid invigilator, ensuring exam integrity through vigilant time-keeping, strict adherence to examination protocols, and maintaining a calm and controlled environment for students.

Education

Doctor of Philosophy (PhD) in Chemistry, Newcastle University Sept 2020 – Dec 2024

Thesis Title: 'Theoretical Insights into Defects and Dynamics in Solid Electrolyte Materials'
Supervisor: Dr James A. Dawson
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 – Jul 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 Title: 'Isotopic Lithium Diffusion in Stoichiometric Solid-State Systems for Lithium Separation'
Supervisor: Dr Samuel T. Murphy
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'
Supervisor: Dr Richard Dawson

- 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 using reverse osmosis principles.
- Applied hazard mitigation and prevention techniques (e.g., HAZID, HAZOP) and implemented key design elements, such as P&IDs.

Publications & Current Research

Disentangling Cation and Anion Dynamics in Li_3PS_4 Solid Electrolytes. **F. N. Forrester**, J. A. Quirk, T. Famprikis, and J. A. Dawson, *Chem. Mater.* **2022**, *34*, 10561–10571. doi.org/10.1021/acs.chemmater.2c02637

Crystalline Crossroads: Impact of Grain Boundaries on Ion Transport and Electronic Structure in Mg Spinels. **F. N. Forrester**, J. A. Quirk, J. M. Hemingway, and J. A. Dawson [*In preparation*]

Comprehensive First Principles Study of Point Defects in Li_3PS_4. **F. N. Forrester**, S. R. Kavanagh, J. A. Quirk, A. Walsh, D. O. Scanlon, and J. A. Dawson [*In preparation*]

Exploration of UX_3-Type Materials as Solid Electrolyte Materials. X. Mao, **F. N. Forrester**, A. Watkins, and J. A. Dawson [*In preparation*]

Unleashing Superionic Conduction in Rare Earth Hydrides. J. A. Dawson and **F. N. Forrester** [*In preparation*]

Professional Memberships

- Associate Fellow of the Higher Education Academy (AFHEA), awarded for meeting UK professional standards in higher education teaching and learning support.
- 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

Referees

Dr James A. Dawson
Reader and Newcastle Academic Track (NUAcT) Fellow in Energy Materials, Newcastle University
Email: james.dawson@newcastle.ac.uk

Dr Samuel T. Murphy
Senior Lecturer in Nuclear Materials and Engineering, Lancaster University
Email: samuel.murphy@lancaster.ac.uk

Tom Harding
School Manager, Natural and Environmental Sciences, Newcastle University
Email: tom.harding@newcastle.ac.uk