Frazer N. Forrester

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

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Profile

An accomplished and highly capable computational materials scientist with interests that lie at the intersection of innovation in **energy**, **environment**, and **engineering**. Currently a Research Assistant in the group of Dr James Dawson at Newcastle University, I utilise atomistic modelling—both quantum and classical—to investigate the role of **defects** and **dynamics** in solid-state systems; with the aim of bridging the gap between theory and application to guide meaningful and targeted research and development.

Skills Overview

- Density Functional Theory (DFT) - Code: VASP
- Classical and *ab initio* Molecular Dynamics - Codes: LAMMPS, GULP
- High-Performance Computing (HPC) – Tiers 1 - 3, working with Slurm and PBS schedulers.
- Python
- Shell Scripting: Bash, Zsh
- Research Management

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, Molecular Dynamics and, more recently, Machine Learning Interatomic Potentials (MLIPs).

- Trained and supervised several PhD and MChem projects—Receiving 5 nominations for Newcastle University's 'The Education Awards (TEAs) 2024'.
- **Research Associate (RA) Committee Member** - representing RA interests and perspectives on school-level committees concerning research, education, management, and EDI.

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

- Gained expertise in both classical and *ab initio* methods of solid-state materials modelling (e.g. GULP, LAMMPS, VASP).
- Pioneered the establishment of research and lab culture within my research group; as the first member, contributed to its growth to over 20 members.
- Implemented and chaired weekly group meetings and tutorial sessions to aid collaboration.
- Established relationships and collaborated with multiple national and international collaborators.
- Designed and supervised multiple MChem projects and PhD students, leading to publication-quality research.
- Proactively identified bottlenecks in the computational workflow and successfully secured regular HPC funding through the EPSRC's Materials Chemistry Consortium (MCC), for resources on Archer 2 (>200,000 CUs).
- Affiliate member of the EPSRC Centre for Doctoral Training in Renewable Energy Northeast Universities (ReNU).

Interim Module Lead, Newcastle University, UK — Dec 2023 – Feb 2023

- Modernised the 'Scientific Computing for Chemists' module with up-to-date techniques and tools, enhancing student engagement and relevance to current chemistry research.
- Demonstrated multiple problem-solving methods to highlight diverse "correct" approaches, fostering critical thinking and adaptability in scientific computing.

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

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

- Taught introductory Python programming, focusing on applications relevant to scientific computing and data analysis.
- Taught multiple characterisation and synthesis techniques (e.g. UV-Vis, Fluorescence, etc.)
- Debugged experimental setups, marked and moderated student work, and delivered formative and substantive feedback.
- Established strong interpersonal relationships with students, academics, and technical staff, fostering a supportive learning environment.

Exam Invigilator, Newcastle University, UK Mayb 2022 – August 2022

Selected as a paid invigilator, responsible for maintaining exam integrity through vigilant time-keeping, adherence to examination protocols, and ensuring a calm, 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 various engineering software and techniques, including, but not limited to HAZID, HAZOP, P&ID, PFD, Aspen, Ansys, and CAD, applied consistently throughout my engineering studies.

Final Year Thesis: '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, including MD and HPC, which contributed to securing a PhD studentship.
- Demonstrated resilience and adaptability in exploring topics beyond the formal curriculum.

Third-Year Design Project: 'Production of Next Generation Ammonia through Direct Electrochemical Synthesis'
Supervisor: Dr Richard Dawson

- Collaborated on route selection and created a comprehensive design report for a plant capable of producing 1000 tonnes/day of next-generation ammonia.
- Independently designed a multi-faceted water purification system based on reverse osmosis from first principles.
- Applied hazard mitigation and prevention techniques (e.g. HAZID, HAZOP) and implemented design aspects 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, 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, 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.
- 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.

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