

Candidate Information

Position:	Research Fellow
School/Department:	Chemistry and Chemical Engineering
Reference:	22/110087
Closing Date:	Monday 29 August 2022
Salary:	£35,333 - £42,155 per annum
Anticipated Interview Date:	Monday 12 September 2022
Duration:	Available until 30 September 2024

JOB PURPOSE:

Applications are invited for a 2-year Research Fellow to work in the group of Dr Paul Dingwall (www.dingwall-lab.co.uk) at Queen's University Belfast. The project involves an in-depth mechanistic study of hypervalent iodine mediated oxidation reactions using a range of highly complementary experimental and computational techniques. A physical organic first approach will involve detailed in situ kinetic and spectroscopic studies. The electrochemical behaviour of the reactions will be investigated in collaboration with the Kavanagh lab (Queen's University Belfast). Computational investigation of the reaction mechanism will be performed with state-of-the-art density functional theory techniques as well as a modern, data driven, physical organic approach to simultaneously probe reaction mechanism and optimise reaction performance. We are looking for a highly motivated individual who is able to bring expertise in at least one of these areas, and who is willing to learn and become an expert in the others. This position is funded by the Leverhulme Trust and is in collaboration with Professor Thomas Wirth (Cardiff University), an additional position on this project in the Wirth Lab will be available early in 2023.

MAJOR DUTIES:

1. Undertake research under supervision within a specific research project or as a member of a research team.
2. Perform kinetic studies on synthetic laboratory-scale reactions either by in situ IR spectroscopy or by sampling and off-line analysis (GC, HPLC, NMR as appropriate).
3. Perform small scale organic synthesis of required materials
4. Perform cyclic voltammetry electrochemical studies
5. Perform density functional theory calculations on a remote high performance cluster running Gaussian 16
6. Utilise Python, and associated tools and libraries, to perform statistical analysis of experimental results
7. Carry out analyses, critical evaluations, and interpretations using methodologies and other techniques appropriate to area of research.
8. Produce high quality research outputs consistent with project aims and commensurate with career stage. This will include collaborating and co-authoring with PI and project team (as appropriate) on outputs.
9. In consultation with the project team, promote research milestones and outputs at national and international conferences.
10. Assist grant holder in the preparation of funding proposals and applications to external bodies.
11. Carry out occasional supervision of more junior colleagues and students in laboratory matters, as well as potential educational supervision, demonstrating or lecturing duties within the post holder's area of expertise and under the direct guidance of a member of academic staff.
12. Undertake supplementary duties relevant to the success of the project including administrative duties and additional training and development activities as required.

ESSENTIAL CRITERIA:

1. Have a degree in Chemistry or a related discipline (minimum standard 2:1)
2. Have, or be about to obtain, a PhD in Chemistry or a related discipline (NB 'About to obtain' is normally defined as within 6 months of application date).
3. At least 3 years relevant research experience of physical organic or synthetic organic chemistry
4. A track record of mechanistic analysis in homogeneous catalysis or organic chemistry.

5. Ability to apply core analytical techniques (1D/2D NMR, MS, IR, HPLC).
6. Working effectively as part of a research team in the development and promotion of the research theme.
7. Ability to supervise more junior colleagues/students in laboratory matters (safety, experimental design, methods), and in the preparation of theses, presentations, reports etc.
8. Ability to contribute to broader management and administrative processes.
9. Contribute to the School's outreach programme by links with industry, community groups etc.
10. Practical problem solving skills, independence of thought and initiative.
11. Ability to assess and organise resources.
12. Ability to communicate complex information in English effectively in oral and written format.
13. Ability to build relationships to develop internal and external networks.
14. Demonstrable intellectual ability.
15. Ability to take a leading role within the research group.
16. Commitment to continuous professional development.

DESIRABLE CRITERIA:

1. Author on publications in peer-reviewed journals.
2. Experience of designing and conducting kinetic experiments.
3. Experience of computational techniques, including the use of Gaussian 16.
4. Experience of electrochemical investigation (voltammetry).
5. Knowledge of programming with Python.
6. Knowledge of data analytical techniques such as multivariate linear regression, principal component analysis, k-means clustering.