

Job Title:	Research Associate in Computational Chemistry
Department/Division/Faculty:	Department of Chemistry, Faculty of Natural Sciences
Campus location:	White City Campus
Job Family/Level:	Research Family, Research Associate*
Responsible to:	Professor Henry Rzepa
Line Management responsibility for:	N/A
Key Working Relationships (external):	Professor Tom Sheppard (UCL), Professor Andy Whiting (Durham), and Dr Jordi Burés (Manchester).
Contract type:	Full-time, Fixed-term for 24 months.

Purpose of the Post

The postholder will be required to carry out computational modelling using Quantum density functional theory of reaction mechanism pathways of novel catalysts for direct amidation reactions. There will be opportunity to learn about and exploit the latest techniques in data management as part of the project, according to modern FAIR data principles. The postholder will work alongside collaborators at UCL, Durham & Manchester who will carry out the design, synthesis and evaluation of novel catalysts for direct amidation reactions and reaction kinetic analysis as part of the same EPSRC-funded project. The research project will build upon recent work on the development of novel catalytic amidation reactions (*Sci. Adv.* **2017**, *3*, e1701028; *Chem. Eur. J.* **2018**, *24*, 7033; *Org. Biomol. Chem.* **2019**, *17*, 6465) and the elucidation of their mechanisms (*Chem. Sci.* **2018**, *9*, 1058; *J. Org. Chem.* **2018**, *83*, 8020).

Key Responsibilities

- You will contribute to the design and discovery of novel organic chemical reactions and synthetic sequences by computational modelling and analysis.
- You will record, analyze and write up the results of the research.
- You will contribute to the drafting and submitting of papers to peer reviewed journals.
- To prepare progress reports on research for funding bodies as required.
- To contribute to the preparation and drafting of research bids and proposals.
- You will contribute to the overall activities of the research team and department as required.
- To undertake a limited amount of teaching in relation to the subject area.
- To contribute to the induction and direction of other research staff and students as requested.

- Responsible for ensuring that equipment is safe and maintained in working order.

*Candidates who have not yet been officially awarded their PhD will be appointed as Research Assistant within the salary range, £35,477- £38,566 per annum.

Person Specification

Requirements	Essential (E)/ Desirable (D)
Candidates/post holders will be expected to demonstrate the following:	
Education	
Research Assistant: Near completion of a PhD in Organic and/or Computational Chemistry	E
Research Associate: Hold a PhD in Organic and/or Computational Chemistry	E
Experience & Knowledge	
Knowledge of research techniques in computational quantum chemistry, including elucidation of potential energy surfaces using quantum mechanical methods.	E
Experience of computer operating systems and programs for computational modelling and display such as Gaussian and Gaussview.	D
Experience of Internet-based search and data management techniques and the authoring of simple Web pages.	D
Experience with one or more of the following: organoboron chemistry; elucidation of reaction mechanisms of organic molecules, computational analysis of NMR, IR spectroscopies, data management techniques.	D
Publications in peer-reviewed international journals commensurate with career stage	E
Skills & Abilities	
Commitment to high quality research	E
Ability to work collaboratively and as part of a team	E
Effective written and verbal communication skills in English	E
Ability to develop and apply new concepts	E
Creative approach to problem-solving	E
Excellent verbal communication skills and the ability to deal with a wide range of people	E
Proven research skills	E
Ability to analyse and write up data	E
Ability to present complex information effectively to a range of audiences	E
Excellent written communication skills and the ability to write clearly and succinctly for publication	E
Ability to organise own work with minimal supervision	E
Ability to prioritise own work in response to deadlines	E
Advanced computer skills, including word-processing, spreadsheets, Internet	E
Other Requirements	
Commitment to maintaining and enhancing facilities and training others in their use	E
Commitment to meeting deadlines	E
Flexible attitude towards work	E
Discipline and regard for confidentiality and security at all times	E
Willingness to undertake any necessary training for the role	E
Willingness to travel both within the United Kingdom and abroad to conduct research and attend conferences/workshops and other meetings	E

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Please note that job descriptions cannot be exhaustive and the post-holder may be required to undertake other duties, which are broadly in line with the above key responsibilities.

Imperial College is committed to equality of opportunity and to eliminating discrimination. All employees are expected to follow the [7 Imperial Expectations](#) detailed below:

- 1) Champion a positive approach to change and opportunity
- 2) Encourage inclusive participation and eliminate discrimination
- 3) Communicate regularly and effectively within and across teams
- 4) Consider the thoughts and expectations of others
- 5) Deliver positive outcomes
- 6) Develop and grow skills and expertise
- 7) Work in a planned and managed way

Employees are required to comply with all College policies and regulations paying special attention to:

- Confidentiality
- Conflict of Interest
- Data Protection
- Equal Opportunities
- Financial Regulations
- Health and Safety
- Information Technology
- Smoking
- Private Engagements and Register of Interests

They must also undertake specific training and assume responsibility for safety relevant to specific roles, as set out on the [College Website Health and Safety Structure and Responsibilities](#) page.

The College is a proud signatory to the San-Francisco Declaration on Research Assessment (DORA), which means that in hiring and promotion decisions, we evaluate applicants on the quality of their work, not the journal impact factor where it is published. For more information, see <https://www.imperial.ac.uk/research-and-innovation/about-imperial-research/research-evaluation/>

The College believes that the use of animals in research is vital to improve human and animal health and welfare. Animals may only be used in research programmes where their use is shown to be necessary for developing new treatments and making medical advances. Imperial is committed to ensuring that, in cases where this research is deemed essential, all animals in the College's care are treated with full respect, and that all staff involved with this work show due consideration at every level.
<http://www.imperial.ac.uk/research-and-innovation/about-imperial-research/research-integrity/animal-research/>

Committed to equality and valuing diversity, we are an Athena SWAN Gold Award winner, a Stonewall Diversity Champion, a Disability Confident Leader and work in partnership with GIRES to promote respect for trans people.

September 2020