



## **Postdoctoral Researcher in Computational Chemistry School of Chemical Sciences**

### **Research Framework – Level 1 Up to 24 Months Full Time Fixed Term Contract**

#### **Research Career Framework**

As part of this role the researcher will be required to participate in the DCU Research Career Framework. This framework is designed to provide significant professional development opportunities to Researchers and offer the best opportunities in terms of a wider career path.

#### **Background & Role**

Dublin City University ([www.dcu.ie](http://www.dcu.ie)) is a research-intensive, globally-engaged, dynamic institution that is distinguished both by the quality and impact of its graduates and by its focus on the translation of knowledge into societal and economic benefit.

The School of Chemical Sciences are seeking to appoint a highly motivated Postdoctoral Researcher to undertake leading edge research in the area of computational chemistry. This research position is funded by Science Foundation Ireland *via* the Synthesis and Solid State Pharmaceutical Centre ([www.sspc.ie](http://www.sspc.ie)). The successful applicant will join a team of researchers at DCU, led by the PI (Dr. Anthony Reilly), exploring new tools and methods for modelling and predicting multi-component pharmaceutical solid forms.

#### **Principal Duties and Responsibilities**

Reporting to his/her Principal Investigator the Postdoctoral Researcher will:

- Conduct a specified programme of research under the supervision and direction of the Principal Investigator. The programme of research will involve developing and applying new modelling tools and methods for predicting the formation and properties (e.g. solubility) of multi-component pharmaceutical solid forms.
- Disseminate the outcomes of the research in which he/she is engaged, including publishing in high quality peer-reviewed journals of international standing, with the support of and under the supervision of the Principal Investigator.
- Support the PI and research group in the design and development and implementation of the research programme.
- Support if required, the development of proposals for research funding.
- Take responsibility, as requested, for day-to-day advice and support of graduate research students and research assistants associated with your research group.
- Mentor, assist and train as appropriate and as directed, more junior research members within the group.
- Contribute to reporting and other administrative management work associated with your

programme of research and the research group, as necessary.

- Engage in appropriate training and development opportunities as required by the Principal Investigator, the School, or the University.
- Contribute to teaching and outreach activities of the research group.
- Liaise with both internal and external stakeholders, including industry and academic partners/collaborators.

### **Minimum Criteria**

- Applicants should have a PhD in Computational Chemistry or Computational Materials Science
- Experience in atomistic modelling of molecular materials
- Strong communication (oral and written) skills, demonstrated by peer-review publications and/or conference presentations

### **Desirable Criteria**

- Experience in one or more of the following atomistic modelling techniques:
  - Density-functional theory
  - Force fields or empirical potentials
  - Density-functional tight binding
  - Crystal structure prediction
- Experience in using machine-learning or informatics approaches for molecules and crystals
- Experience in using python
- Experience in supporting project management and reporting, as well as interactions with academic and industrial collaborators

**Salary:** €37,874–€38,417

Appointment will be commensurate with qualifications and experience will be made on the appropriate point of the salary scale, in line with current Government pay policy.

**Closing date:** Friday 13<sup>th</sup> September, 2019

**Candidates will be assessed on the following competencies:**

**Discipline knowledge and Research skills** – Demonstrates knowledge of a research discipline and the ability to conduct a specific programme of research within that discipline.

**Understanding the Research Environment** – Demonstrates an awareness of the research environment (for example funding bodies) and the ability to contribute to grant applications.

**Communicating Research** – Demonstrates the ability to communicate their research with their peers and the wider research community (for example presenting at conferences and publishing research in relevant journals) and the potential to teach and tutor students.

**Managing & Leadership skills** - Demonstrates the potential to manage a research project including the supervision of undergraduate students.

**Informal enquiries to:**

*Dr. Anthony Reilly, School of Chemical Sciences, DCU, Glasnevin, Dublin 9*

*E-mail: anthony.reilly@dcu.ie*

*Phone: +353 (0)1 7006709*

**Application Procedure**

To apply for this role, application forms are available from the DCU Current Vacancies (open Competitions) website at <http://www.dcu.ie/vacancies/current.shtml> and also from the Human Resources Department, Dublin City University, Dublin 9. Tel: +353 (0) 1 7005149.

**Please clearly state the role that you are applying for in your application and email subject line: Job Ref #RF1268 Postdoctoral Researcher in Computational Chemistry**

*Applications should be submitted by email to [hr.applications@dcu.ie](mailto:hr.applications@dcu.ie) or by Fax: +353 (0)1 7005500 or by post to the Human Resources Department, Dublin City University, Dublin 9. Human Resources Department, Dublin City University, Dublin 9. Tel: +353 1 700 5149; Fax: +353 1 700 5500 Email: Insert [hr.applications@dcu.ie](mailto:hr.applications@dcu.ie)*

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