

## Candidate Information

<b>Position:</b>	Research Fellow
<b>School/Department:</b>	Biological Sciences
<b>Reference:</b>	21/109161
<b>Closing Date:</b>	Monday 4 October 2021
<b>Salary:</b>	£34,304 - £40,927 per annum
<b>Anticipated Interview Date:</b>	Wednesday 13 October 2021
<b>Duration:</b>	2 Year Fixed-Term Contract

### JOB PURPOSE:

The post holder will be engaged in an exciting interdisciplinary research project investigating the bio-catalytic formation of gas hydrates. This academic project involves close collaboration with biochemists, computational physicists and chemical engineers – led by Professor Chris Allen and Professor Niall English (University College Dublin) and will ultimately lead to inter-disciplinary publication at an international level.

The position will entail the molecular-dynamics (MD) simulation of gas-hydrate formation and crystallisation, in contact with, and adsorbed atop, biological catalysts, such as protein surfaces. There will be very close synergy for MD simulation with allied laboratory experiments.

The successful candidate will have a demonstrable track record in: non-equilibrium MD, in the presence of externally applied fields, e.g., magnetic; code development (Fortran, C, Python) and order-parameter analysis (e.g., Steinhardt, CHILL); MD engines (NAMD, GROMACS, DL-POLY), as well as writing own code and modifying community codes.

### MAJOR DUTIES:

1. Undertake research under supervision to investigate the bio-catalytic formation of gas hydrates within a specific research project.
2. Design, develop and refine experiments in order to obtain reliable data.
3. Carry out analyses, critical evaluations, and interpretations using methodologies and other techniques appropriate to area of research.
4. Present regular progress reports on research to members of the research group or to external audiences to disseminate and publicise research findings.
5. Prepare, often in consultation with supervisor, material for publication in national and international journals and presentations at international conferences.
6. Assist grant holder in the preparation of funding proposals and applications to external bodies.
7. Carry out routine administrative tasks associated with the research project/s to ensure that project/s are completed on time and within budget. These might include organisation of project meetings and documentation, financial control, risk assessment of research activities.
8. Carry out occasional undergraduate supervision, demonstrating or lecturing duties within the post holder's area of expertise and under the direct guidance of a member of academic staff.
9. Read academic papers, journals and textbooks to keep abreast of developments in own specialism and related disciplines.
10. Assist with supervision of undergraduate/postgraduate research appropriate to expertise.

### Planning and Organising:

1. Plan for specific aspects of research programmes. Timescales range from 1-12 months in advance and contribute to research group planning.
2. Plan for the use of research resources, laboratories and workshops where appropriate.
3. Plan own day-to day activity within framework of the agreed research programme.
4. Plan up to a year in advance to meet deadlines for journal publications and to prepare presentations and papers for conferences.

5. Coordinate and liaise with other members of the research group over work progress.
6. Make regular visit to collaboration group based at University College Dublin for meetings and to assist with research activities.

**Resource Management Responsibilities:**

1. Ensure research resources are used in an effective and efficient manner.
2. Provide guidance as required to support staff and any students who may be assisting with research.

**Internal and External Relationships:**

1. Liaise on a regular basis with colleagues and students.
2. Build internal contacts and participate in internal networks for the exchange of information and to form relationships for future collaboration.
3. Join external networks to share information and ideas.
4. Contribute to the School's outreach programme by establishing links with local community groups, industries etc.

**ESSENTIAL CRITERIA:**

1. Honours degree at 2.2. or equivalent in physics, chemistry, chemical engineering, biochemistry, biophysics or related discipline.
2. Have or be about to obtain a PhD in a relevant area to the job description – for example, containing a major component of MD simulation experience either relating to biological or non-biological systems.
3. At least 3 years recent relevant research experience to include a minimum of 2 years:
  - MD simulation research, related to ordering/crystallisation events
  - Code development (Fortran, C, Python) and order-parameter analysis (e.g., Steinhardt, CHILL)
  - Writing own code and/or modifying community codes.
4. Display an active interest in the application of MD methods to solving bio-molecular research problems.
5. Publication record commensurate with stage of career.
6. Ability to contribute to broader management and administrative processes.
7. Sufficient breadth and depth of specialist knowledge in the discipline and of research methods and techniques to work within established research programmes.
8. Ability to communicate complex information clearly.
9. Ability to build contacts and participate in internal and external networks.
10. Demonstrable intellectual ability.
11. Ability to assess and organise resources.

**DESIRABLE CRITERIA:**

1. 6 months minimum experience of:
  - non-equilibrium MD research.
  - MD engines (NAMD, GROMACS, DL-POLY)
2. Free-energy and biased-simulation methods including PLUMED.
3. Biomolecular-simulation.
4. HPC, GPU, parallel-computing, sys-admin and compilation skills
5. Protein structure analysis.
6. Co-author in an academic publication.
7. Using and maintaining Linux supercomputer operation environment.