

## Candidate Information

<b>Position:</b>	Research Fellow
<b>School/Department:</b>	School of Mathematics and Physics
<b>Reference:</b>	19/107257
<b>Closing Date:</b>	Tuesday 26 March 2019
<b>Salary:</b>	£33,199 - £34,189 per annum
<b>Duration:</b>	one year

### JOB PURPOSE:

To be an active member of the NSF-SFI-DfE research project "ThermoConc" assisting in the planning and delivery of the research activity within the field of computational modelling of thermoelectric transport processes in construction materials, so that the overall research objectives of the project/school are met.

### MAJOR DUTIES:

1. Undertake basic research activities within the field of computational modelling of thermoelectric transport processes in cement, especially in the vicinity of metallic fibers. Develop a mesoscale model of a concrete mixture to predict and validate its thermoelectric properties against experimental data.
2. Integrate microscopic Density functional Theory (DFT) calculations and experimental data with finite element macroscopic models of full cement bricks.
3. Present regular progress reports on research to members of the research group and to external audiences to disseminate and publicise research findings. Participate and present the work in international conferences.
4. Write up results of own work and contribute to the production of research reports, publications and proposals.
5. 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.
6. Develop a collaborative relationship with partners at TU Dublin (Dublin, Rol), Purdue University (Indiana, USA), and Washington University in St. Louis (Missouri, USA), and travel to meet the partners as required.
7. Carry out any other duties designated by the line manager and which fall within the general remit of the post.
8. Regularly assist with supervision of graduate and undergraduate students involved in related projects, and contribute to postgraduate supervision within this project.
9. May carry out undergraduate supervision/demonstrating/teaching duties under direction.

### Planning and Organising:

1. Plan own day-to-day activity within the framework of the agreed research programme.
2. Contribute to the planning of research projects, reports and publications.
3. Coordinate and liaise with other members of the research group in Ireland and USA over work progress.

### 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 research colleagues and support staff on routine matters.
2. Build internal and external contacts and participate in networks to develop knowledge and to form relationships for future collaboration.
3. Attend and contribute to relevant seminars and meetings.

4. Participate in the design and coordination of training activities for PhD students in the Atomistic Simulation Centre and in the ThermoConc consortium.

**ESSENTIAL CRITERIA:**

1. PhD in Physics, Chemistry, Engineering, or related subject. Must have qualification conferred by institution on or before the commencement date.
2. 3 years' relevant research experience to include Experience in computer simulation of complex materials at the atomic scale.
3. Demonstrable publication record in international refereed journals, commensurate with experience.
4. Sufficient breadth and depth of specialist knowledge in the discipline and of research methods and techniques to work within the established research programme.
5. Ability to communicate complex information clearly.
6. Excellent written and verbal communication skills.
7. Demonstrable intellectual ability.
8. Good interpersonal skills and ability to collaborate and interact with colleagues.
9. Willing to interact with colleagues in Dublin, Purdue and St. Louis.
10. Willing to travel and spend some time in partner locations - Dublin, Purdue and St. Louis.

**DESIRABLE CRITERIA:**

1. Training in Computational Physics/Chemistry
2. Training in Finite Elements modelling
3. Practical experience in electronic structure methods, especially DFT, and ab initio molecular dynamics.
4. Experience in modelling cementitious materials.
5. Experience in finite element modelling and COMSOL multiphysics
6. Knowledge of Python programming language
7. One or more years relevant postdoctoral research experience.
8. Experience of knowledge transfer from fundamental to applied research and engineering.
9. Ability to assess and organise resources