

# **Candidate Information**

Position: School/Department: Reference: Closing Date: Salary:

Anticipated Interview Date: Duration:

Research Fellow School of Mathematics and Physics 18/106754 Tuesday 25 September 2018 £33,199 - £39,610 per annum (potential to progress to £43,266 per annum through sustained exceptional contribution) Tuesday 16 October 2018 3 years

## 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 research activities within the field of computational modelling of thermoelectric transport processes in cement, especially in the vicinity of metallic fibres, including set up and carry out simulations using first-principles DFT approaches, interpret and analyse the results.
- 2. Utilise and further develop a methodology to obtain transport coefficients from DFT results, using Boltzmann's equation. Interface microscopic models with finite element macroscopic models of full 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 DIT (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 ambit 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, usually 1-6 months in advance.
- 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 be in possession of the qualification by the commencement date. (Must have been awarded PhD by commencement date)
- 2. Minimum three years relevant research experience
  - To include Experience in electronic structure methods and computer simulation
- 3. 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. Excellent verbal and written communication skills.
- 6. Demonstrable intellectual ability.
- 7. Good interpersonal skills
- 8. Willing to travel to partner sites to work with colleagues in Dublin, Purdue and St.Louis, as necessary.

## DESIRABLE CRITERIA:

- 1. Training in Solid State Physics/Chemistry
- 2. Training in Computational Physics/Chemistry
- 3. Training in Physical Chemistry
- 4. Experience in DFT simulations of complex materials, especially cement.
- 5. Experience in calculation of thermoelectric properties of materials.
- 6. Experience in transport calculations using Boltzmann's equation.
- 7. Publications in top quartile journals.
- 8. 2 years relevant postdoctoral research experience.
- 9. Knowledge of modelling of construction materials and engineering structures
- 10. Ability to assess and organise resources