# JOB DESCRIPTION

| | |
|---|---|
| **Vacancy reference:** | SRF33501 |
| **Post Title:** | Postdoctoral Researcher in Computational Solid-State Chemistry |
| **Grade:** | Grade 6 |
| **School/Department:** | Chemistry |
| **Reports to:** | Prof. A.V. Powell |
| **Responsible for:** | N/A |

## Purpose

The role holder will carry out a research program in computational solid-state materials chemistry on a project to investigate materials for thermoelectric energy harvesting. The project is funded through the EPSRC Global Challenges Research Fund initiative and seeks to develop new solid-state materials for the extraction of electrical power from traditional Indian cookstoves (chulhas).

## Main duties and responsibilities

The principal duties will include:

- Computer simulation of electron and phonon structure in copper-based materials, including those based on the chalcopyrite, chalcocite and bornite structures. This will involve the use of density functional theory as implemented in codes like VASP, Quantum Espresso, etc.
- Theoretical estimation of charge transport coefficients using Boltzmann's transport theory and suitable approximations for the electron-phonon coupling. This will involve the use of codes like BoltzTrap or BoltzWann.
- Theoretical estimation of lattice heat transfer coefficients from the computation of anharmonic forces in the materials, using codes like ShenBTE, phono3py, etc.
- Theoretical estimation of the thermoelectric figure of merit of the investigated materials based on calculated transport coefficients at different levels of doping and as a function of temperature.
- Liaison with both experimental and theoretical researchers at other academic partner institutions.
- Presentation of results at regular review meetings of the project team and at selected conferences and workshops.
- Preparation of results for publication.
- Contribute to the writing of papers for publication in leading academic journals and other relevant media

**Supervision received**

The project will be supervised by Dr R Grau-Crespo and Prof. A.V. Powell.

**Supervision given**

No formal supervision will be given. Informal support to other members of the research group may be given.

**Contact**

This is part of an EPSRC-funded project involving collaboration between University of Reading, University of Manchester and the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India.

**Terms and conditions**

This post is offered on a full-time, fixed term basis of up to 16 months. There are no specific hours of work, but the appointee will be required to work such hours as are necessary to carry out the duties associated with the post.

This document outlines the duties required for the time being of the post to indicate the level of responsibility. It is not a comprehensive or exhaustive list and the line manager may vary duties from time to time which do not change the general character of the job or the level of responsibility entailed.

**Date assessed:** 21 August 2020

# PERSON SPECIFICATION

| Job Title | School/Department |
|---|---|
| **Postdoctoral Researcher in Computational Solid-State Chemistry** | **Chemistry/SCFP** |

| Criteria | Essential | Desirable |
|---|---|---|
| **Skills Required** | • Expertise in computational solid-state chemistry or physics.<br>• Ability to work with codes for density functional theory calculation of the electronic structure of solids (VASP, Quantum Espresso, WIEN2k or similar).<br>• Excellent critical analysis skills<br>• Good oral and written communication<br>• Ability to work to deadlines | • Ability to use software for the calculation of electron transport properties (BoltzTrap, BoltzWann, etc).<br>• Ability to use software for the calculation of lattice thermal conductivity (ShengBTE, phono3py, etc).<br>• Basic programming skills (scripting languages or Fortran). |
| **Attainment** | • First or upper second-class honours degree or equivalent in chemistry, physics or a related discipline.<br>• A PhD (or soon to complete) in computational chemistry or physics or in materials chemistry.<br>• A good publication record for level of experience | • . |
| **Knowledge** | • Knowledge of density functional theory and quantum chemistry.<br>• Understanding of electron band structure in solids<br>• Understanding of phonon structure in solids | • Understanding of electron and phonon transport process in solids.<br>• Knowledge of thermoelectric phenomena. |
| **Relevant Experience** | • Postgraduate experience in computational solid-state science or materials chemistry gained during a doctoral degree. | • Experience working in high-performance computing environments.<br>• Prior experience of multi-organization research projects.<br>• Experience collaborating with experimentalists. |
| **Disposition** | • Disposition and ability to work independently, but also collaboratively with team members at all levels, in a multi-organization project.<br>• Strongly motivated with good organisational skills.<br>• Good interpersonal skills | • |

| | |
|---|---|
| Completed by: Dr. R. Grau-Crespo and Prof. A.V. Powell | Date: 21/08/2020 |