



## **Project Title**

### **Barocaloric organic ionic plastic crystals and prototype development**

A PhD studentship is available in the group of Dr Claire L. Hobday (School of Chemistry, The University of Edinburgh; (<http://www.chem.ed.ac.uk/staff/academic-staff/dr-claire-hobday> ) in collaboration with Sunamp, UK (<https://sunamp.com/#home/>).

This PhD project corresponds to the Doctoral Candidate no. UK1 (DCUK1) vacancy notice of the MSCA “Molecule-based magneto-/electro-/mechano-calorics” (MolCal) Doctoral Network composed of 8 beneficiaries and 6 associated partners from France, Germany, Greece, Italy, Netherlands, Spain, United Kingdom and United States. MolCal overarching scientific goal is the preparation of new molecular assemblies with outstanding potential as caloric materials for refrigeration and heat pump applications at near-ambient and very-low temperature, and their exploitation in prototype devices.

The successful candidate will enrol in the PhD degree programme in Chemistry at the University of Edinburgh and be employed for 36 months within MolCal. This multidisciplinary and multisectoral network with strong research and training excellence, will ensure optimal knowledge transfer via shared hosting and joint supervision. A personalised career development plan will be established to support the needs of the candidate.

## **We offer**

The gross salary (not including social security deductions) will be £ 33,195-42,773 per annum plus mobility (£ 5,359 per annum) and family allowances (£ 5,984) as applicable and in-line with the EC rules for MSCA Doctoral Networks 2022. The studentship is fully funded for 36 months for a candidate satisfying EPSRC residency criteria. <https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/#contents-list>

## **Project Summary**

Solid-state materials have the potential to increase refrigeration efficiency, as well as replacing outdated greenhouse gas vapour-compression technology. Globally, refrigeration accounts for 17 % of electricity usage, so there is an exciting materials chemistry challenge to replace inefficient and harmful gases with solid-state refrigerants. Refrigerant effects can be induced in solids through the application of an external field which causes a change in entropy and temperature to the system, named caloric solids. This innovative field is still in its infancy, with recent research work focused on magneto- or electro- caloric effects. The application of hydrostatic pressure to induce barocaloric effects (BCE) is much less studied but offers the most promising advancement as a safer and less energy intensive alternative.

This doctoral project targets the determination of the structural and thermal origins of the BCE. A combination of experimental and computational approaches will be used to get a holistic view of the BCE. High-pressure diffraction and calorimetry will be used to help establish how order-disorder transitions drive refrigeration effects. The project will make use of central facilities such as Diamond Light Source and The European Synchrotron Radiation Facility for in-situ diffraction studies. The structural and thermal data will be used to help model the system via molecular dynamics simulations and machine learning models to help improve the caloric materials synthesised within the MolCal partners. The selected DC will be enrolled and based at the School of Chemistry, The University of Edinburgh. There will also be secondments with experienced MolCal partners at Sunamp Ltd. in

MacMerry (United Kingdom; D. Oliver) and CSIC in Zaragoza (Spain; M. Evangelisti) for high-pressure calorimetry.

### **We seek**

The candidate should have a strong background in materials characterisation or molecular simulation, with a Master's degree in Chemistry or related fields. Further information for PhD enrolment at The University of Edinburgh, including English language requirements, can be found [here](#).

Specific eligibility criteria of the Horizon Europe MSCA programme apply, including:

PhD status: applicants must not already be in possession of a doctoral degree at the date of the recruitment.

Mobility rule: applicants must not have resided or carried out their main activity in the country of the host organisation for more than 12 months in the 3 years immediately before their recruitment date.

### **How to apply**

In the first instance, the initial application (including cover letter outlining your suitability for the PhD, transcripts and CV) should be directed to:

Dr Claire L. Hobday, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK.  
Claire.Hobday@ed.ac.uk

The position will remain open until 21<sup>st</sup> April 2024.

Additional information is available on the MolCal website <https://molcal.eu/dcs/>

### **IMPORTANT**

Before Submitting your cover letter, transcripts and CV, please complete the online [School of Chemistry Equality, Diversity and Inclusion Form 2024](#).

**The form will automatically generate a unique “Receipt Number” that you MUST include in your cover letter.**

### **Equality and Diversity**

The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality. The University has a range of initiatives to support a family friendly working environment. See our University Initiatives website for further information. University Initiatives website: <https://www.ed.ac.uk/equality-diversity/help-advice/family-friendly>