

## **PhD position. Development of a meta-heuristic algorithm for MOF crystal structure prediction**

A PhD project at Nottingham Trent University (UK) and Université de Poitiers (France) is available in the development of a meta-heuristic algorithm for MOF crystal structure prediction (starting date: september 2023). This joint PhD thesis is supervised by Dr. Matthew Addicoat (NTU) and Dr. Gilles Frapper (IC2MP, UP).

**Overview.** Functional porous materials based on two- and three-dimensional coordination polymers are conceptually the result of a fantastic Lego game. Indeed, their crystalline framework is the result of the arrangement of elementary components: a metal site, associated with a (redox) ligand, and a counter-ion inserted into the cavities of the metal-ligand framework. The intimate association of these three components metal, ligand and counter-ions, in a key-lock type game, modulates the material's physico-chemical properties: crystallinity, network topology, conducting behaviour, magnetic order, catalytic activity, etc. Exploring the possibilities of such an ensemble by usual methods, whether experimental or theoretical, is dizzying. A change of paradigm is thus required.

In this joint project between Nottingham Trent University and Université de Poitiers, France, which will lead to a Dual Award PhD, we propose to elaborate a methodology to design and develop Functional Metal Organic Frameworks (MOFs) by an intelligent exploration of the whole set of possibilities issuing from combinations of metal/ligand/counter ions. We will extend and integrate the AuToGraFS structure builder with the XTalOpt evolutionary algorithm and machine-learned potentials to build a fully open-source multi-component MOF structure search platform. Then, we will focus on the prediction of new MOFs with designed properties thanks to selected fitness functions (band gap, thermoelectric, magnetism...).

The candidate should have some skills in programming languages (Python, Fortran, C/C++) and Linux; an experience in CSP methodology and MOF modeling is a plus (e.g., random/evolutionary algorithms). A good knowledge of written and spoken English is essential to communicate at both UK and France labs and with external collaborators. PhD manuscript and defense will be in english.

Applicants should hold, or be expected to hold, an UK Master's degree or France Master's degree (or UK / Fr equivalent according to NARIC) with a minimum of a commendation, and/or a UK 1stClass / 2.1 Bachelor's Honour's Degree (or UK equivalent according to NARIC).

For further information about the project and the application procedure (EXTENDED deadline) please visit: <http://ntu.ac.uk/research/find-a-phd-opportunity/projects/science-technology/development-of-a-meta-heuristic-algorithm-for-mof-crystal-structure-prediction>

Send your CV and motivation letter to: Dr Matthew Addicoat [matthew.addicoat@ntu.ac.uk](mailto:matthew.addicoat@ntu.ac.uk) and Dr Gilles Frapper [gilles.frapper@univ-poitiers.fr](mailto:gilles.frapper@univ-poitiers.fr)

## **Fees and funding**

Joint project between Nottingham Trent University (18 months) and Université de Poitiers (18 months), France, which will lead to a Dual Award PhD. The project is a fully funded at UKRI level / CNRS including a 3 year stipend (~1700 € net salary, CNRS contract funded by ANR).