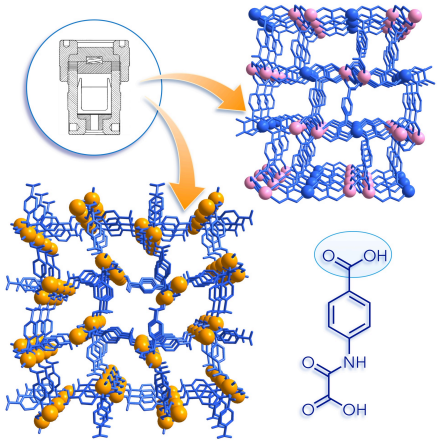
Available PhD studentship:

Reactivity of oxamate ligands in solvothermal and microwave synthetic conditions: *preparing MOFs for molecule sensing or ion mobility.*

Institut Parisien de Chimie Moléculaire — Sorbonne Université
ERMMES Group.
Supervisors: L. Lisnard, A. Flambard and R. Lescouëzec.
Start date: Oct. 2nd 2023.



Oxamate ligands are the source of numerous molecular materials with an impressive range of applications and properties: water remediation, sieving, sensing, catalysis or magnetism.[1–4] The search for novel forms of oxamate ligands and the coordination architectures they yield is inherently related to these successes and stress the importance of investigative synthetic work. In the group, we are investigating multi-polydentate ligands where a phenyloxamate scaffold is augmented with hydroxo or carboxylato coordinating groups. The study of their reactivity with 3d metal ions has successfully led to new structural morphologies and we have also demonstrated that solvothermal synthetic conditions are advantageous in the crystallisation process.[5–8]

We aim in the course of this project to extend our synthetic approach and orient the preparation of our networks towards two important fields of study in MOF chemistry: molecule sensing and ion mobility. Regarding the former, our next synthetic goal is the controlled preparation of neutral networks possessing a physicochemical response appropriate to the detection of molecules. We will tune the starting materials' charge in solvothermal conditions (3d metal ions oxidation number, nature and number of the additional coordinating groups on the phenyloxamate scaffold) and develop microwave synthetic conditions to increase the reactivity of our ligands, while preventing their degradation. To detect the molecule, two strategies will be used, both involving a magnetic response: the preparation of magnets or the formation of switchable networks with the introduction of spin crossover centres in the framework. Regarding ion mobility, we will focus on our charged networks, and evaluate them on their conduction properties (protons, alkaline and multivalent ions) within the frame of a pre-existing collaboration (PHENIX lab in Sorbonne Université). More specifically, we target intercalation materials for applications in battery.

This project includes: bench organic and inorganic synthesis for the preparation of the starting materials; coordination chemistry in solvothermal and microwave conditions for the preparation of the networks; solution and solid-state NMR, solution and solid-state UV-Vis, FT-IR, powder X-ray diffraction, single-crystal X-ray diffraction, thermodiffraction, TGA, and SQUID magnetometry for the characterisation of the compounds and the study of their properties.

We are seeking a highly motivated student with a keen interest in developing skills both in synthetic coordination chemistry and multi-technique physicochemical characterisations. Candidates should hold or be about to obtain a master's degree in chemistry or materials science.

Contact details:

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Deadline for application: May 12th 2023. Guidelines:
http://www.ed406.upmc.fr/fr/contrats-doctoraux/depot-des-candidatures.html

1 T. Grancha, et al. *Chem. Commun.*, 2014, **50**, 7569–7585.
2 M. Castellano, et al. *Coord. Chem. Rev.*, 2015, **303**, 110–138.
3 F. R. Fortea-Pérez, et al. *Nat. Mater.*, 2017, **16**, 760–766.
4 M. Mon, et al. *J. Mater. Chem. A*, 2018, **6**, 4912–4947.
5 A. Li, et al. *Eur. J. Inorg. Chem.*, 2020, **2020**, 3311–3319.
6 A. Li, et al. *Dalton Trans.*, 2021, **50**, 681–688.
7 A. Li, et al. *Inorg. Chim. Acta*, 2021, **521**, 120320.
8 A. Li, et al. *Cryst. Growth Des.*, 2022, **22**, 7518–7526.