

## ESR 4 position

### Project title: pH-dependent uptake and release of guest molecules from a coordination cage

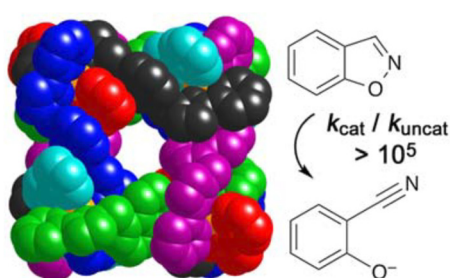
Location: University of Warwick, UK

Supervisor: Prof. Michael Ward

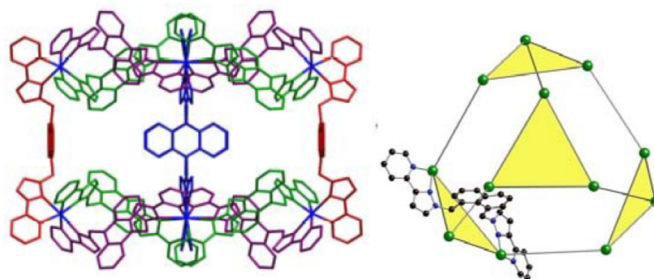
#### Objectives of the individual project:

This PhD project is part of the European Training Network 'NOAH' (Network of functional molecular containers with controlled switchable abilities) that has received funding from the European Union's Horizon 2020 programme.

This project concerns a range of hollow metal/ligand capsules ('coordination cages') which are hollow, and contain central cavities that can bind small-molecule 'guests' inside them. These cages have hydrophilic exteriors and are water-soluble, but have hydrophobic interior cavities which provide the basis for strong guest binding. The consequences of guest binding include catalysis of reactions of bound guests; size- and shape-selective luminescent sensing; and the ability to transport molecular 'cargoes'.



**Fig. 1.**  $10^5$ -fold catalysis of an elimination reaction in the cavity of a coordination cage



**Fig. 2.** Illustrative examples of other types of coordination cage architecture based on the same ligand family

The scientific project will involve the preparation and structural characterisation of new members of the coordination cage family and the evaluation and quantification of guest binding in the cage cavity by a combination of molecular modelling and spectroscopic measurements. In particular, the ability to control guest uptake and release using external stimuli such as pH changes or an applied redox potential will be developed as the basis of new types of functional behaviour, because the control of guest binding and release is fundamental to a wide range of applications. In catalysis, the starting material must bind strongly but the product must be released to allow a second cycle; and for transport applications, it is necessary for the 'carrier' to be able to bind and release its 'cargo' on demand.

The work is highly multi-disciplinary and will include elements of organic and inorganic synthesis; a range of characterisation methods such as NMR spectroscopy, mass spectrometry and X-ray crystallography and physical / analytical techniques such as luminescence spectroscopy and kinetic measurements to probe the properties of the host / guest systems. The 36-month project will include a 3-month secondment to a partner institution in Germany to perform mass spectrometric analyses of cage/guest systems, and a 6-month secondment to technological centre in Spain to study recyclable molecular containers for encapsulation of drugs for skin regeneration.

Representative recent publications illustrating the work are as follows:



W. Cullen, A. J. Metherell, A. B. Wragg, C. G. P. Taylor, N. H. Williams, M. D. Ward, *J. Am. Chem. Soc.*, 2018, 140, 2821.

C. G. P. Taylor, W. Cullen, O. M. Collier, M. D. Ward, *Chem. Eur. J.*, 2017, 23, 206.

W. Cullen, M. C. Misuraca, C. A. Hunter, N. H. Williams, M. D. Ward, *Nature Chem.*, 2016, 8, 231.

W. Cullen, S. Turega, C. A. Hunter, M. D. Ward, *Chem. Sci.*, 2015, 6, 625.

S. Turega, W. Cullen, M. Whitehead, C. A. Hunter, M. D. Ward, *J. Am. Chem. Soc.*, 2014, 136, 8475.

### Planned secondment(s):

**Academic Secondment:** 3-months secondment to discover the potential of mass spectrometry techniques for quantitative thermodynamic measurements at FUB (Germany).

**Industrial Secondment:** Six-months secondment at LEITAT facilities in Spain in order to work on recyclable molecular containers for encapsulation and skin regeneration.

### Eligibility requirements

**EU eligibility criteria for candidates:** Candidates of any nationality, but in order to be eligible for the positions the following criteria applies to all applicants:

- The applicant shall at the time of recruitment be in the **first four years of his/her research career** and have **not been awarded a doctoral degree**.
- The applicant must not have resided or carried out his/her main activity in **UK for more than 12 months in the 3 years immediately prior to the recruitment**.

**Candidates profile:** candidates must hold a **Master's degree in Chemistry** with excellent academic transcripts. We are looking for **highly motivated** students with **good communication skills**

All candidates must **prove full proficiency in spoken and written English** (B2 certificate, TOEFL, or equivalent).

Questions regarding the recruitment can be sent to: [noah@noah-itn.eu](mailto:noah@noah-itn.eu).

Questions regarding the project can be sent to: [M.D.Ward@warwick.ac.uk](mailto:M.D.Ward@warwick.ac.uk)

