

A 3.5-year PhD studentship in “Novel Catalysts based on Metal-Containing Molecular Containers”

Supervisors: Dr. Tung Chun Lee (UCL), Dr. Shiqiang Bai (IMRE, A*STAR)

Closing Date for Applications: 30 June 2018

Start Date: 24 September 2018

Location: London (1.5 years), Singapore (2 years)

Topics: nanomaterials, catalysis, reaction mechanism, supramolecular chemistry, host-guest complexes

The Studentship

This position is fully funded by the UCL-A*STAR Collaborative Programme via the Centre for Doctoral Training in Molecular Modelling and Materials Science (M3S CDT) at UCL. The student will be registered for a PhD at UCL where he/she will spend year 1 and the first six months of year 4. The second and third years of the PhD will be spent at the A*STAR Institute of Materials Research and Engineering (IMRE) in Singapore. The Studentship will cover tuition fees at UK/EU rate plus a maintenance stipend £17,050 (tax free) pro rata in years 1 and 4. During years 2 and 3, the student will receive a full stipend directly from A*STAR. In addition, A*STAR will provide the student with one-off relocation allowance. **Please note that, due to funding restrictions, only UK/EU citizens are eligible for this studentship.**

The Project

Enzymes are known to speed up a wide variety of chemical reactions through encapsulating small molecular species into their nanoscale cavities (a.k.a. the enzymatic pockets) and in many cases stabilising the transition states of a reaction via metal-ligand interactions at the active sites. Our group has demonstrated that the nanoscale cavities of artificial molecular containers (cucurbit[*n*]urils CB*n*) can mediate cascades of chemical reactions, analogous to enzymatic pockets.^[1] Owing to their well-defined and controllable molecular structures, CBs can serve as an excellent model system for studying enzymatic and other inner-phase reactions, as well as for designing more efficient catalysts.

This PhD project aims to develop novel catalysts that mimic the function of enzymes, which will synergise with other experimental and modelling effort led by the Lee group. In particular, highly selective and efficient catalysts will be achieved by combining the molecular recognition properties of CBs with the catalytic properties of transition metal ions, metal nanoparticles and semiconductor quantum dots. The project aims to develop a molecular toolbox that enables bespoke catalysts to be assembled through a mix-and-match approach, and to deliver fundamental insights into reaction mechanisms within a nano-confined environment.

Please visit the group website for more details about our research: <http://tungchunlee.weebly.com/>

[1] “Chemistry inside molecular containers in the gas phase”, *Nat. Chem.*, **2013**, *5*, 376–382.

The Candidate

The successful applicant should have or expect to achieve a 1st or 2:1 class integrated Masters degree (MEng, MSci, MChem etc.) in Chemistry, Physics, Materials Science, or a related discipline. The successful applicant will demonstrate strong interest and self-motivation in the subject, good experimental practice and the ability to think analytically and creatively. Good computer skills, plus good presentation and writing skills in English, are required. Previous research experience in contributing to a collaborative interdisciplinary research environment is highly desirable but not necessary as training will be provided.

Please contact Dr. Tung Chun Lee (tungchun.lee@ucl.ac.uk) for further details or to express an interest.

Applications will be accepted until **30 June 2018** but the position will be filled as soon as an appropriate candidate is found.