A 3.5-year PhD studentship in "Mechanism of Catalysis inside Nanoreactors"

Supervisors: Dr. Tung Chun Lee (UCL), Dr. David O. Scanlon (UCL), Dr. Yong-Wei Zhang (IHPC, A*STAR)

Closing Date for Applications: 15 June 2017

Start Date: September 2017

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

Topics: supramolecular chemistry, host-guest complexes, chemical reaction mechanism, catalysis, computer-aided discovery, molecular modelling, density functional theory (DFT), ab initio molecular dynamics (AIMD)

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 High Performance Computing (IHPC) in Singapore. The Studentship will cover tuition fees at UK/EU rate plus a maintenance stipend £16,553 (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

Understanding the mechanism of how molecules react in chemical catalysis is of interest because it can lead to more efficient chemical processes. For instance, in catalyses that involve encapsulation of reactant molecules within a nanoscale cavity (i.e. a "nanoreactor", as found in zeolites, metal-organic framework and enzymes), it is known that the reaction rate of a specific pathway can be enhanced if the intermediate species are stabilised by interaction with the cavity wall. Nevertheless, the role of nano-cavities in catalytic mechanism is largely unexplored because it is difficult to isolate and study the highly unstable, short-lived reaction intermediates within the "inner phase", let alone to correlate a number of intermediates throughout a reaction cascade.

This PhD project aims to deliver by **computational methods** quantum mechanical understanding of chemical reactions inside molecular nanoreactors, which will complement and synergise with the experimental effort led by the Lee group.[1] Promising molecular systems for both experiments and simulations will be identified via computer-aided discovery approaches. Design rules for exotic chemistry in supramolecular and catalytic systems will be obtained through computational investigation into selected host-guest complexes using first principle techniques, e.g. density functional theory (DFT) and ab initio molecular dynamics (AIMD).

Please visit our group websites for more details about our research:
http://tungchunlee.weebly.com/
http://davidscanlon.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 computational 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) or Dr. David O. Scanlon (d.scanlon@ucl.ac.uk) for further details or to express an interest.

Applications will be accepted until 15 June 2017 but the position will be filled as soon as an appropriate candidate is found.