

## **A 3-Year PhD Studentship in “Supramolecular Upconversion of van der Waals Interaction Energy” (D/L:15/04/2023)**

Supervisors: Dr. Tung Chun Lee (UCL), Dr. Qiang Zhu (IMRE, A\*STAR, Singapore)

Application deadline: 15/04/2023

Interview date: TBC (2 to 4 weeks after the application close date)

Start date: 25 September 2023

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

Subject areas: Supramolecular chemistry, host-guest complexes, catalysis, organic synthesis, chemical reaction mechanism, energy conversion, high-throughput screening, molecular modelling

### **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 in IMRE of A\*STAR in Singapore. The studentship will cover tuition fees at the home rate, and an annual stipend of no less than £19668 increasingly annually with inflation (tax free) pro rata in years 1 and 4. During years 2 and 3, the student will receive a stipend of S\$2700 per month directly from A\*STAR. In addition, A\*STAR will provide the student a one-off relocation allowance.

### **The Project**

Harvesting energy from van der Waals (vdW) interactions, e.g. hydrogen bonding, and other intermolecular effects, e.g. hydrophobic effects, to produce energy-rich molecules is of fundamental interests, due to the universal nature of such interactions. Nevertheless, achieving this type of energy upconversion can be a daunting task because vdW forces are 10–100 times weaker than a chemical bond. An effective approach to minimise energy mismatch and thus to enhance energy conversion efficiency is (1) to identify a molecular system that exhibits strong vdW interactions and (2) to couple it to chemical reactions with a small change in free energy  $\Delta G$ .

This PhD project aims to develop **novel experimental approaches** of supramolecular upconversion of vdW interaction energy, which will synergise with other experimental and modelling effort led by the Lee group. In particular, efficient energy conversion will be achieved by designing molecular structures of reactive guests via simultaneously optimising their host-guest binding affinity and reaction thermodynamics. Success of the project will open new possibilities in systems chemistry and may even allow us to construct dissipative systems far from thermodynamic equilibrium. It will also have implications on energy harvesting in nanosystems and nanodevices where means of power supply remain limited.

Please visit our websites for more details about our research:

<http://tungchunlee.weebly.com/>

<https://www.a-star.edu.sg/imre/research-departments/advanced-characterization-and-instrumentation>

### **The Candidate**

The applicants should have, or be expecting to achieve, a first or upper second-class integrated Masters degree (MSci, MChem, MEng etc.) or a 2:1 minimum BSc plus a stand-alone Masters degree with at least a Merit 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.

Interested candidates should initially contact Dr. Tung Chun Lee ([tungchun.lee@ucl.ac.uk](mailto:tungchun.lee@ucl.ac.uk)) with a CV, a degree transcript and a motivation letter expressing interest in the project. Informal inquiries are encouraged.

Please note that a suitable applicant will first be required to complete [MS Form](#) entitled Application for Research: degree Chemistry programme. In addition, it is essential that suitable applicants complete an electronic application form at <https://www.ucl.ac.uk/prospective-students/graduate/research-degrees/chemistry-mphil-phd> (Select Research degree: Chemistry programme) prior to the application deadline and advise their referees to submit their references as soon as they possibly can. All shortlisted applicants will be invited for an interview no more than 4 weeks after the application deadline. Any admissions queries should be directed to Dr. Zhimei Du via [z.du@ucl.ac.uk](mailto:z.du@ucl.ac.uk)

Applications are welcome from UK nationals and EU nationals with settled/pre-settled status. Please note that the studentship only covers home fees. The updated rules for eligibility for home fees for next year are available at [View Website](#).

Applications will be accepted until 15/04/2023.