

PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
School	School of Science
Supervisors	<p><i>Please list all the names in the supervisory team. It should be consistent with the information on your approved PGRS proposal.</i></p> <p>Principal supervisor: Dr. Lifeng Ding (XJTLU) Co-supervisor: Dr. Linjiang Chen.....(University of Birmingham) Co-supervisor: Dr. Haifei Zhang.....(UoL)</p>
Application Deadline	Open until the position is filled
Funding Availability	Funded PhD project (world-wide students)
Project Title	Exploring MOFs for Ammonia Storage as an Alternative Hydrogen Carrier using GCMC and Machine Learning Methods
Contact	<p>Please email Lifeng.Ding@xjtlu.edu.cn (XJTLU principal supervisor's email address) with a subject line of the PhD project title.</p> <p>The principal supervisor's profile is linked here: https://www.xjtlu.edu.cn/en/departments/academic-departments/chemistry/staff/lifeng-ding</p>

Requirements:

The candidate should have a first class or upper second class honours degree, or a master's degree (or equivalent qualification), in Chemistry, Computational Chemistry, Material Science, Physics or Mathematics.

Evidence of good spoken and written English is essential. The candidate should have an IELTS score of **6.5 or above**, if the first language is not English. This position is open to all qualified candidates irrespective of nationality.

Degree:

The student will be awarded a PhD degree from the University of Liverpool (UK) upon successful completion of the program.

Funding:

The PhD studentship is available for three years subject to satisfactory progress by the student. The award covers tuition fees for three years (currently equivalent to RMB 99,000 per annum). It also provides up to RMB 16,500 to allow participation at international conferences during the period of the award. The scholarship holder is expected to carry out the major part of his or her

research at XJTLU in Suzhou, China. However, he or she is eligible for a research study visit to the University of Liverpool up to six months, if this is required by the project.

Project Description:

The challenge of hydrogen storage has long been acknowledged due to its flammability and low energy density. In light of this, ammonia (NH₃) has emerged as a promising alternative hydrogen storage medium, characterized by high energy density and stability. In this study, we aim to investigate the use of metal-organic frameworks (MOFs) as a solid NH₃ storage medium. MOFs offer large structural diversity, featuring large surface area and tunable pore structures. Through a combination of molecular simulation and machine learning (ML), this study will study two large MOF databases to identify those with high NH₃ deliverable storage capacity. This research will yield a comprehensive understanding of the fundamental mechanisms governing NH₃ storage in MOFs and establish the groundwork for the development of efficient NH₃ storage materials for use in renewable energy applications.

For more information about doctoral scholarship and PhD programme at Xi'an Jiaotong-Liverpool University (XJTLU), please visit

<https://www.xjtlu.edu.cn/en/admissions/global/entry-requirements/>

<https://www.xjtlu.edu.cn/en/admissions/global/fees-and-scholarship>

How to Apply:

Interested applicants are advised to email Lifeng.Ding@xjtlu.edu.cn (XJTLU principal supervisor's email address) the following documents for initial review and assessment (please put the project title in the subject line).

- CV
- Two formal reference letters
- Personal statement outlining your interest in the position
- Certificates of English language qualifications (IELTS or equivalent)
- Full academic transcripts in both Chinese and English (for international students, only the English version is required)
- Verified certificates of education qualifications in both Chinese and English (for international students, only the English version is required)
- PDF copy of Master Degree dissertation (or an equivalent writing sample) and examiners reports available