PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
School	School of Sciene
Supervisors	Principal supervisor: Dr. Lifeng Ding (XJTLU) Co-supervisor: Dr Zhenghao Wu (XJTLU) Co-supervisor: Professor Alessandro Troisi (UoL)
Application Deadline	Open until the position is filled
Funding Availability	Funded PhD project (world-wide students)
Project Title	Computer-Aided Discovery of Photo-Responsive Metal Organic Frameworks for Energy Efficient CO_2 Capture
Contact	Please email Lifeng.Ding@xjtlu.edu.cn (XJTLU principal supervisor's email address) with a subject line of the PhD project title. The principal supervisor's profile is linked here: https://scholar.xjtlu.edu.cn/en/persons/LifengDing

Requirements:

A Master's degree with Merit and a Bachelor's degree with first-class or upper second-class honors are required for PhD admissions. Exceptional candidates holding only a Bachelor's degree may be considered on an individual basis in certain disciplines.

Evidence of good spoken and written English is essential. The candidate should have an IELTS (or equivalent) score of 6.5 or above, if the first language is not English. This position is open to all qualified candidates with Chemistry, Material Science/Engineering, Physics, Artificial Intelligence background, 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 holders are expected to conduct the majority of their

research at XJTLU in Suzhou, China. However, they may apply for a short-term research visit to the University of Liverpool if the project requires it.

Project Description:

The rising atmospheric CO_2 level necessitates the development of advanced carbon capture technologies. Nanoporous materials with their high surface area and tunable pore structures, are promising candidates for CO_2 capture. However, the energy-intensive cyclic CO_2 adsorption and desorption processes remain a significant barrier to their wide use. This proposal aims to address this challenge by optimizing MOFs with photo-responsive properties, enabling energy-efficient light control to regulate CO_2 capture and release processes. By employing computational techniques such as Machine Learning, Grand Canonical Monte Carlo (GCMC) simulations and density functional theory (DFT), this research will design and screen photo-responsive MOFs for enhanced CO_2 capture. A high-throughput screening of large MOF database will be conducted, with top-performing materials selected for experimental validation under varying light conditions to confirm computational predictions.

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