PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
Academy	Academy of Life and Natural Sciences
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 Simulation Driven Porous Material Database Construction for External Field Responsive CO_2 Adsorbents
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:

Porous materials such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), hydrogen-bonded organic frameworks (HOFs), and porous organic cages (POCs) have attracted significant attention for carbon dioxide (CO_2) capture due to their high surface areas, tunable porosity, and chemical versatility. However, most existing materials databases primarily catalog static structural information and neglect the influence of external fields—such as electric fields, mechanical stress, or temperature gradients—on adsorption performance, despite the fact that such stimuli can significantly modulate gas uptake, selectivity, and diffusion behavior. Moreover, many reported frameworks are computationally optimized without considering realistic deformation or flexibility, which are critical under operational conditions. To address these limitations, this project will systematically construct and simulate new porous frameworks, accounting for their structural response and performance under external fields through a fully computational approach, thereby creating a comprehensive and dynamic porous material database to support the rational design of next-generation field-responsive CO_2 adsorbents.

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