PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
School	School of Science
Supervisors	Principal supervisor: Dr. Lifeng Ding (XJTLU) Co-supervisor: Professor John Dennis (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 Porous Materials for the Purification of Fullerene Adducts
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:

The candidate should have a first class or upper second class honours degree, or a master's degree (or equivalent qualification), in Chemistry, Physics, Chemical Engineering, Electronic Engineering or Material Science. Priorities will be given to candidates with computational chemistry background.

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:

Fullerenes and their adducts find extensive applications, particularly as electroactive materials in solar cells, and continue to emerge in new medical uses. However, their broad utility is hindered by labor-intensive solid-liquid extractions, typically in toluene, and time-consuming chromatographic separations. Recent advancements explore the host-guest chemistry of molecular containers for fullerene encapsulation, aiming to overcome selectivity challenges associated with fine modulation of molecular cage size in covalent synthesis. The proposed research project, focusing on identifying novel porous materials for the separation of fullerene homologue pairs, holds immense potential value and impact across scientific, industrial, and technological domains. The outlined objectives and methodologies promise to address critical challenges in fullerene enrichment and separation, opening avenues for practical applications and innovations. Here, we delve into the potential value and impact of each aspect of the proposed research.

(1). Overcoming Practical Limitations in Fullerene Production: The proposed research directly addresses this bottleneck by aiming to identify suitable porous materials for the separation of different fullerene. The successful execution of the computational strategy holds the promise of overcoming these practical limitations, resulting in enhanced fullerene production, which is crucial for advancements in various fields, including materials science, electronics, and pharmaceuticals.

(2). Innovative Screening Workflow for Fullerene Separation: Through the innovative high-throughput in-silico screening (molecular dynamics simulations and Density Functional Theory calculations) approach the resulting top-performing porous materials, identified through this workflow, not only advance the field of gas separation in porous materials but also offer experimental validation, contributing to the reliability and applicability of the screening strategy.

(3). Unveiling Structure-Function Correlations through Machine Learning: The qualitative and quantitative correlation between porous materials' structures and their ability to separate fullerenes, represents a significant leap in understanding how porous materials recognize fullerene adducts. Machine learning models trained on data from existing porous materials can also forecast separation performance, and aligns with the broader goals of materials informatics, offering a systematic approach to designing advanced materials tailored for specific 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…....@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