PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
School	School of Science (Department of Chemistry)
Supervisors	*Please list all the names in the supervisory team. It should be consistent with the information on your approved PGRS proposal.* Principal supervisor: Dr. Zhenghao Wu (XJTLU) Co-supervisor: Dr. Lifeng Ding (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	Machine Learning for Multiscale Simulations of Polymers with First-Principal Accuracy
Contact	Please email zhenghao.wu@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/ZhenghaoWu https://wuresearchgroup.github.io/

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/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:
Molecular simulations have become an invaluable tool in the development of polymer science and engineering. Inherently constrained by their complexity, the application of common molecular simulation methods for predicting the behavior of polymer systems is however not entirely satisfactory and therefore novel methods are needed particularly for simulations at large spatio-temporal scales. Recently, the integration of machine learning (ML) into the realm of computational chemistry has ushered in a new era of scientific progress, overcoming the longstanding challenges posed by the computational intricacies associated with conventional quantum and molecular mechanical approaches. This project aims to develop a general and consistent multiscale molecular simulation framework for polymeric materials with first-principle accuracy using advanced ML techniques, holding the potential to advance our theoretical and computational infrastructure for accelerating polymeric materials design.

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 zhenghao.wu@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