

### PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
School	School of Science
Supervisors	Principal supervisor: Professor Heechae Choi (XJTLU) Co-supervisor: Professor Li Yang (XJTLU) Co-supervisor: Dr Danlei Li (XJTLU) Co-supervisor: Professor Xin Tu (UoL)
Application Deadline	Open until the position is filled
Funding Availability	Funded PhD project (world-wide students)
Project Title	Photo- and electro-catalyst designs using combination of electrochemistry and electrodynamics implemented in multi-scale simulations
Contact	Please email Heechae.Choi@xjtlu.edu.cn (XJTLU principal supervisor's email address) with a subject line of the PhD project title

#### **Requirements:**

The candidate should have a first class or upper second class honours degree, or a master's degree (or equivalent qualification), in ..... 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) and provides a monthly stipend of 5,000 RMB as a contribution to living expenses. It also provides up to RMB 16,500 to allow participation at international conferences during the period of the award. It is a condition of the award that holders of XJTLU PhD scholarships carry out 300-500 hours of teaching assistance work per year. 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 of up to six months, if this is required by the project.

### **Project Description:**

Eco-friendly energy conversion technology is very promising and in a high demand. In the last two decades, energy conversions using catalysts have shown a tremendous growth with the aids of computational chemistry. The current catalyst designs largely rely on the state-of-art first-principles (quantum mechanical) calculations, which are giving accurate molecule binding energies on catalysts. In this project, a successful candidate is going to primarily perform atomic-scale modeling and simulations using density functional theory (DFT) and/or molecular dynamics (MD) simulations. Optionally, catalysts design principle will be developed by the successful candidate by utilizing classical electrodynamics and fluid dynamics in order to take into accounts the electrostatic forces and ion transport.

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 reference letters with company/university letterhead
- Personal statement outlining your interest in the position
- Proof of English language proficiency (an IELTS score of 6.5 or above)
- Verified school 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

**Informal enquiries** may be addressed to Professor Heechae Choi (Heechae.Choi@xjtlu.edu.cn), whose personal profile is linked below,

<https://www.xjtlu.edu.cn/en/staff-details/staff/heecheae-choi>