PhD studentship (Full-time)

Institution	Xi'an Jiaotong-Liverpool University, China
Schoo	School of Science
Supervisors	Principal supervisor: Professor Heechae Choi (XJTLU) Co-supervisor: Dr Tianhong Gu (XJTLU) Co-supervisor: Dr Shuihua Wang (XJTLU) Co-supervisor: Professor Jianliang Xiao (UoL)
Application Deadline	May 31st, 2025
Funding Availability	Funded PhD project (world-wide students)
Project Title	Noble-Metal Free High-Entropy Alloy Catalyst Design for Drug Synthesis Driven by Machine Learning
Contact	Please email Tianhong.Gu@xjtlu.edu.cn and/or Heechae.Choi@xjtlu.edu.cn with a subject line of the PhD project title. The supervisor's profiles are linked here: https://scholar.xjtlu.edu.cn/en/persons/TianhongGu https://scholar.xjtlu.edu.cn/en/persons/HeechaeChoi

Requirements:

1. The candidate should have an undergraduate degree with first-class or upper second-class honours and a master's degree (or equivalent qualification) in materials science or relative fields in chemistry, physics, and chemical engineering.
2. 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.
3. Knowledge of crystal structure, phase transformation, and solidification kinetics.
4. Capabilities of alloy design, material processing, and using material characterisation, e.g. XRD, DSC, SEM (EDS+EBSD), S/TEM, FIB, etc.
5. Experience in using computational tools (physico-chemical criteria, computational thermodynamics Calphad / Thermo-Calc, physical solid solution hardening model).

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:

This research aims to design and optimize cost-effective, non-precious metal high-entropy alloy (HEA) catalysts for the Heck reaction in drug synthesis by leveraging Density Functional Theory (DFT) and machine learning algorithms. This involves collecting adsorption data on pure metal surfaces to analyze catalytic properties and interactions relevant to the Heck reaction. Machine learning algorithms will be employed to analyze this data, identify patterns, and propose optimal HEA compositions that enhance catalytic efficiency and stability. The proposed HEA catalysts will be validated through further DFT calculations and laboratory experiments to confirm their predicted performance. Additionally, the study aims to compare the catalytic performance of optimized HEAs with traditional precious metal catalysts to quantify the degree of improvement in drug synthesis applications.

The candidate will design alloys using both experiments and computational methods (Calphad / Thermo-Calc, physical solid solution hardening model) in collaboration with catalyst research teams from XJTLU and partner universities from the UK, South Korea, Japan, and Germany.

Research Questions:

- Adsorption Properties and Catalysis: What are the adsorption properties of pure metal surfaces, and how do these properties correlate with catalytic performance in the Heck reaction?
- Optimal HEA Element Combinations: Which combinations of 4-5 elements in HEAs provide the highest stability and catalytic efficiency for the Heck reaction in drug synthesis?
- Role of Machine Learning in Catalyst Design: How can machine learning algorithms enhance the prediction of optimal HEA compositions based on adsorption calculation data from the Heck reaction?
- Performance Enhancement of HEA Catalysts: To what extent do optimized HEAs improve catalytic performance compared to traditional precious metal catalysts in the Heck reaction?
- DFT and Machine Learning Prediction Accuracy: How accurate are DFT calculations and machine learning predictions in designing new HEA catalysts for the Heck reaction in drug synthesis when compared with experimental results?

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 Tianhong.Gu@xjtlu.edu.cn and Heechae.Choi@xjtlu.edu.cn (XJTLU supervisors) 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