

### XJTLU-XJTU-UoL Joint Doctoral Supervision Project (Full-time)

Reference No.	<b>SFXJTU2539</b>
XJTLU School	School of Science
PhD Programme	Chemistry
Supervisors	XJTLU supervisor: Dr. Graham Dawson XJTU supervisor: Professor Guoping Gao UoL supervisor: Dr. Alex Neale XJTLU co-supervisor: Dr. Qiuchen Dong
Project Title	Understanding the influence of electron transfer on proton transport in the electric double layer using the fixed-potential method 恒电位电子输运对双电层中质子迁移的影响及机制研究
Application Deadline	Open until the position is filled

#### **Requirements:**

A UK first-class or upper second-class honours Bachelor's degree and a UK Master's degree with Merit (or their equivalent) are required for PhD admissions. Exceptional candidates holding only a Bachelor's degree may be considered on an individual basis.

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.

For more information about entry requirements and admission procedures of PhD programme at XJTLU, please visit:

[Entry Requirement - Xi'an Jiaotong-Liverpool University](#)

[How to Apply - Xi'an Jiaotong-Liverpool University](#)

#### **Programme Structure:**

Doctoral students in the joint programme are registered with both XJTLU and the UoL. Upon successful completion of the programme, the students will be awarded a PhD degree from University of Liverpool.

During their doctoral studies at XJTLU, students are expected to conduct research at XJTU as visiting students. Additionally, students have the opportunity to apply for a three to six-month research visit to UoL.

#### **Project Description:**

The migration of hydrogen protons within the electric double layer serves as a critical "logistics and supply" step in most electrochemical energy storage reactions. Investigating their migration behavior can not only reveal new mechanisms of electrochemical energy storage reactions but

is also particularly important for addressing key technical challenges in fields such as designing high-performance catalysts and exploring interfacial processes in multi-scale, multi-component complex electrochemical systems. As the simplest charged ion in electrochemical reactions, hydrogen protons play essential roles in mass transfer and charge/energy exchange in key carbon-neutral energy storage reactions, such as electrolytic water splitting for hydrogen production, electrochemical CO<sub>2</sub> reduction, and electrochemical ammonia synthesis. Furthermore, the migration rate of hydrogen protons within the electric double layer directly determines the overall efficiency of the energy storage reaction. Therefore, studying the migration behavior of hydrogen protons in the electric double layer is fundamental for understanding the microscopic kinetic properties of electrochemical reactions. Building on our recent work on the hydrogen evolution reaction, this project will employ the grand canonical fixed potential method to investigate the influence of voltage on key physicochemical properties, such as the molecular structure of the electric double layer on a Pt(111) electrode surface, the energy barrier for water molecule reorganization, the energy barrier for hydrogen proton hopping, and the charge exchange between the electrolyte and the electrode during hydrogen proton migration. The aim is to provide guidance for addressing factors that limit hydrogen proton migration in electrochemical reactions.

双电层中质子迁移和体系与外电路之间电子输运将影响整个还原反应的选择性和能量转换机制。然而，恒电位下双电层中质子迁移是否会诱导电极与电源之间的电子输运，以及电子输运行为对质子迁移的影响机制尚不明确。本项目拟以金属与水组成的双电层为主要研究对象，发展优化基于第一性原理的巨正则固定电势法，解决传统第一性原理电化学模拟方法在恒电位质子迁移过程中体系与外电路之间电子输运行为难以模拟的难题，沿着双电层中质子迁移与电子输运之间的耦合行为这一主线，首先研究外电位对质子迁移过程中体系与外电路之间电子输运行为的影响，阐明质子迁移过程中电子-质子耦合协同转移机制；然后通过不同晶面、金属材料、界面水结构来探索电极材料功函数和界面水偶极矩对电子-质子之间耦合关系的影响。最终综合量化外电势、功函数和界面水偶极矩对质子迁移率的贡献，深入了解双电层中质子迁移行为，为改善质子迁移过程中发热耗能问题提供理论支撑。

#### **Joint Supervisory Team:**

XJTLU supervisor: Dr. Graham Dawson

XJTU supervisor: Professor Guoping Gao

UoL supervisor: Dr. Alex Neale

XJTLU co-supervisor: Dr. Qiuchen Dong

#### **How to Apply:**

Interested applicants are advised to email [graham.dawson@xjtlu.edu.cn](mailto:graham.dawson@xjtlu.edu.cn) the following documents for initial review and assessment (Please include 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