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

Reference No.	SFXJTU2529
XJTLU School	School of Advanced Technology
PhD Programme	Computer Science and Software Engineering
Supervisors	XJTLU supervisor: Dr Yushan Pan Co-Supervisor: Prof. Zhijie Xu XJTU supervisor: Professor Pinghui Wang UoL supervisor: Professor Xiaowei Huang
Project Title	Research on Spatiotemporal Graph Neural Networks for AI for Science 面向 AI for Science 的时空图神经网络研究
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

Other Requirements (if any):

N/A

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:

AI for Science (artificially intelligent-driven scientific research) has emerged as a global interdisciplinary frontier in artificial intelligence development. Aiming to leverage AI models for learning scientific principles, discovering scientific laws, and addressing scientific problems, it is hailed as the "fifth paradigm" of scientific research. Notable advancements have been widely recognized by academia and industry in fields such as drug discovery, materials design, and high-energy physics.This project intends to focus on drug molecular dynamics prediction and structure generation as scientific applications to investigate spatiotemporal graph neural network (STGNN) models. Centered on "spatiotemporal dynamics" and "graph (relational) structures" as core analytical objects, the model's universality stems from two fundamental laws: "The world is material, and matter is in motion" (spatiotemporal law) and "Everything is universally connected" (relational law). The specific research contents are outlined as follows:(1) 3D Geometric Attribute Graph Modeling and Representation Learning3D geometric attribute graph modeling is designed to convert spatially structured molecules into computer-processable data structures. Representation learning aims to compress molecular information—including spatial geometry, topological relationships, and chemical properties—into low-dimensional, continuous, and task-agnostic embedding vectors while preserving information completeness.(2) Mechanism-Data Dual-Driven Spatiotemporal Dynamics PredictionSpatiotemporal dynamics prediction focuses on modeling the evolutionary laws of molecular systems across time and space, which is of great significance for tasks such as protein folding and ligand binding. This project proposes a hierarchical spatiotemporal graph neural network model based on logical and mechanistic representations to achieve accurate prediction of molecular dynamics.(3) Geometric Diffusion Models for Molecular Structure GenerationThis research aims to develop geometric diffusion models for generating target-specific molecular structures. Guided by conditions such as desired molecular properties or specific docking conformations, the model will generate valid and interest-aligned 3D molecular structures. Additionally, interpretable attribution methods will be employed to verify the rationality of the generated structures.

AI for Science（人工智能驱动的科学研究）已成为全球人工智能发展的学科交叉前沿，旨在利用 AI 模型学习科学原理，发现科学规律，解决科学问题，被誉为科学研究的第五范式，已在药物发现、材料设计、高能物理等领域取得了学界和业界普遍认可的进步。本课题拟以药物分子动力学预测与结构生成为科学应用，研究时空图神经网络模型。该模型以“时空”与“图（关联）”为主要分析对象，建模的普适性源自两条普遍规律：“世界是物质的，物质是运动的”（时空规律）、“事物是普遍联系的”（关联规律）。本课题具体的研究内容包括：（1）三维几何属性图建模与表示学习方法三维几何属性图建模用于将具有空间特性的分子存储为计算机可处理的数据结构。表示学习旨在保证分子的空间、拓扑和属性等信息完备的条件下，利用深度学习模型将其压缩为低维、连续、任务无关的表示向量。（2）机理数据双驱动的时空动力学预测方法时空动力学预测拟研究预测分子系统在时间和空间上的演变规律，对蛋白质折叠、配体结合等

任务均具有重要意义。本项目拟研究基于逻辑和机理表示的层次时空图神经网络模型，实现对分子动力学的准确预测。（3）面向分子结构生成的几何扩散模型研究本课题拟发展几何扩散模型来生成特定兴趣的分子结构。以特定分子性质或特定对接结构为生成条件，指导模型生成产生有效的、感兴趣的三维分子结构，并利用可解释归因方法验证生成结构的合理性。

Joint Supervisory Team:

XJTLU supervisor: Dr. Yushan Pan (IEEE M’22, SM’24) grew up in Xi’an, China. After completing his studies there, he spent the subsequent twelve years in Norway—pursuing academic endeavors, building his professional career, and laying down roots. This Nordic educational system, which shares similarities with Germany’s higher education model, equipped him with a strong foundation to become a accomplished researcher and educator following the completion of his PhD and Habilitation. In 2022 he returned to China and joined Xi’an Jiaotong-Liverpool University, where he now investigates the sweet spot of Cognitive Intelligence. Before XJTLU, Yushan was a doctoral researcher at the University of Oslo(2013-2017) and later a senior researcher at the Norwegian University of Science and Technology and the Norwegian Maritime Competence Center (2017-2021). He also spent time at Parametric Technology Corporation as a technical consultant (2011-2013). He is also serving as a Senior Member of IEEE, ACM, and CCF, and as a life member of the Chinese Association of Automation. His curiosity roams from emotional AI and cognitive computing to industrial defect spotting, liveness detection, hyperspectral imaging, and trustworthy AI.

潘昱杉博士（IEEE 会员，2022 年当选；IEEE 高级会员，2024 年当选）出生并成长于中国西安。在西安完成学业后，他前往挪威深造、立业、定居，历时十二载。北欧的高等教育体系与德国模式颇为相似，正是在这一体系的培养下，潘博士在取得博士学位并完成大学任教资格认证后，奠定了扎实的学术基础，成长为一名卓有成就的科研与教育工作者。 2022 年，潘博士归国并加入西交利物浦大学，目前致力于认知智能领域的前沿研究。入职西交利物浦大学前，他于 2013—2017 年在奥斯陆大学担任博士研究员；随后于 2017—2021 年，先后在挪威科技大学及挪威海事能力中心担任高级研究员。此外，他还曾于 2011—2013 年任职于参数技术公司，担任技术顾问。 潘博士目前同时担任电气和电子工程师协会（IEEE）、美国计算机协会（ACM）及中国计算机学会（CCF）高级会员，亦是中国自动化学会终身会员。他的研究兴趣广泛，涵盖情感人工智能、认知计算、工业缺陷检测、活体检测、高光谱成像及可信人工智能等多个方向

Co-supervisor: Professor Zhijie Xu is Head of the Department of Computing at XJTLU. Before joining XJTLU in 2024, he worked as a Full Professor specializing in visual computing at the University of Huddersfield in the United Kingdom. During that time, he undertook undergraduate and postgraduate curriculum development and teaching duties across a wide range of computer science and engineering subjects,

including computer graphics, computational geometry, games and extended reality (VR/AR/MR/XR), digital image processing, and computer vision, as well as various team-and-studio-based projects. His research spans over 30 years and delves into real-time graphics, interactive visualization, machine vision, robotics, smart systems, computational linguistics, machine learning, and computer architecture. He has supervised over 20 PhD students to successful completion, published 200 peer-reviewed papers, and edited 5 books. He holds a dozen vision and visualization-related patents, ranging from new algorithms and models to devices and apparatus. He has led, co-led, and peer-reviewed major projects for funding councils such as RCUK and Horizon Europe. He has personally led projects with a total funding of over 1.5 million pounds. Additionally, he has served as an editor for several journals and chaired many conferences.

许志杰教授现任西交利物浦大学计算机系主任，国家部委国家级杰出人才。2024 年加入西交利物浦大学之前，他曾任英国哈德斯菲尔德大学全职教授，专攻视觉计算领域。任职期间，他承担了计算机科学与工程多个学科的本科及研究生课程开发与教学工作，涵盖计算机图形学、计算几何、游戏与扩展现实（VR/AR/MR/XR）、数字图像处理、计算机视觉等方向，同时负责各类团队式及工作室项目的指导工作。徐志杰教授拥有 30 余年研究经验，研究领域广泛，深耕实时图形学、交互式可视化、机器视觉、机器人技术、智能系统、计算语言学、机器学习及计算机体系结构等多个方向。他已指导 20 余名博士生顺利毕业，发表同行评审论文 200 余篇，主编著作 5 部；持有十余项视觉与可视化相关专利，覆盖新算法、新模型、设备装置等多个维度。他曾牵头、联合牵头多项重大科研项目，并担任英国研究理事会（RCUK）、“欧洲地平线”计划等资助机构重大项目的同行评审专家，个人牵头项目累计获得经费超 150 万英镑。此外，他还曾担任多家学术期刊编委，主持过多个国际学术会议。

XJTU supervisor: Prof. Wang Pinghui is a recipient of the National Science Fund for Excellent Young Scholars. He currently serves as Vice Dean of Research at the School of Cyber Science and Engineering, Faculty of Electronic and Information Engineering, Xi’an Jiaotong University, as well as Professor and Doctoral Supervisor at the School of Automation Science and Engineering, Faculty of Electronic and Information Engineering, Xi’an Jiaotong University. He continued his doctoral education at the same university from September 2006 to March 2012 and earned his Doctor’s degree upon graduation. From January 2014 to March 2015, he worked as a Research Fellow at Noah’s Ark Laboratory, Huawei Technologies Co., Ltd. He then served as a Distinguished Research Fellow at Xi’an Jiaotong University from April 2015 to May 2019. In May 2019, he was appointed Professor at the School of Automation Science and Engineering, Faculty of Electronic and Information Engineering, Xi’an Jiaotong University, and in August 2022, he took up the position of Vice Dean of Research at the School of Cyber Science and Engineering, Faculty of Electronic and Information Engineering, Xi’an Jiaotong University. His primary research interests focus on interdisciplinary fields including network big data and cybersecurity.

王平辉教授是国家优秀青年科学基金获得者。他现任西安交通大学电子与信息学部网络空间安全学院科研副院长，同时担任该校电子与信息学部自动化科学与工程学院教授、博士生导师。 2006 年 9 月至 2012 年 3 月，他于本校继续深造，攻读博士学位并顺利毕业。2014 年 1 月至 2015 年 3 月，任华为技术有限公司诺亚方舟实验室研究员；2015 年 4 月至 2019 年 5 月，任西安交通大学特聘研究员；2019 年 5 月，受聘为西安交通大学电子与信息学部自动化科学与工程学院教授；2022 年 8 月，出任西安交通大学电子与信息学部网络空间安全学院科研副院长。 他的主要研究方向聚焦于网络大数据、网络安全等交叉学科领域。

UoL supervisor: Prof. Xiaowei Huang (UoL) is in the Department of Computer Science at the University of Liverpool and leads the Trustworthy Autonomous Cyber Physical System Lab. The research his group is currently conducting spans machine learning, formal methods, and robotics. His research focuses on trustworthy AI, with expertise in verification, explainable AI, and AI safety and security.
利物浦大学的黄晓伟教授任职于该校计算机科学系，同时担任可信自主信息物理系统实验室主任。他所带领的研究团队当前的研究领域涵盖机器学习、形式化方法与机器人学三大方向。黄教授的研究方向聚焦于可信人工智能，在验证技术、可解释人工智能及人工智能安全与防护领域拥有深厚的专业造诣。

How to Apply:

Interested applicants are advised to email Yushan.Pan@xjtlu.edu.cn and/or phwang@mail.xjtu.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