

## 國立清華大學第 29 屆新進人員研究獎得獎人簡介



林昆翰博士自 2022 年起擔任國立清華大學化學工程學系助理教授，研究專長為跨尺度材料模擬，結合第一原理計算、分子動力學及動態蒙地卡羅等方法，從微觀尺度解析材料結構、動力學與功能之間的關係。研究涵蓋有機半導體、光電材料、光催化與電催化等領域，並特別著重以分子模擬理解實驗中難以直接觀察的微觀機制，進而提出材料設計方向。

加入清華後，林教授積極建立獨立研究團隊，並與國內外實驗團隊密切合作，將理論模擬應用於多項能源與功能材料研究。近年以通訊作者身分於 *Journal of the American Chemical Society*、*Nature Communications*、*Science Advances*、*Advanced Functional Materials* 及 *Chemistry of Materials* 等國際期刊發表研究成果，主題涵蓋有機發光二極體、有機太陽能電池、高分子光催化產氫系統及高熵合金電催化觸媒等。

林教授亦重視跨領域與國際合作，自 2023 年起主持德國馬克斯普朗克學會 Max Planck Partner Group，延續與 Max Planck Institute for Polymer Research 的長期合作。未來將持續發展跨尺度模擬方法，以微觀機制為基礎，加速有機光電、催化與能源領域之材料設計與開發。

Dr. Kun-Han Lin has been an Assistant Professor in the Department of Chemical Engineering at National Tsing Hua University (NTHU) since 2022. His research focuses on multiscale materials simulation, integrating first-principles computations, molecular dynamics simulations, and kinetic Monte Carlo methods to elucidate the relationships among material structure, dynamics, and function at the microscopic level. His research spans organic semiconductors, optoelectronic materials, photocatalysis, and electrocatalysis, with particular emphasis on using molecular simulations to uncover microscopic mechanisms

that are difficult to observe directly in experiments and to translate these insights into materials design strategies.

Since joining NTHU, Professor Lin has actively established an independent research group and developed close collaborations with experimental teams in Taiwan and abroad, applying theoretical simulations to a broad range of energy and functional materials. In recent years, he has published research as a corresponding author in international journals including the *Journal of the American Chemical Society*, *Nature Communications*, *Science Advances*, *Advanced Functional Materials*, and *Chemistry of Materials*. These studies cover organic light-emitting diodes, organic solar cells, polymer photocatalytic hydrogen evolution systems, and high-entropy-alloy electrocatalysts.

Professor Lin also places strong emphasis on interdisciplinary and international collaboration. Since 2023, he has led a Max Planck Partner Group, continuing his long-term collaboration with the Max Planck Institute for Polymer Research. Looking forward, his group will continue to advance multiscale simulation methods and, based on a molecular-level understanding of microscopic mechanisms, accelerate the design and development of materials for organic optoelectronics, catalysis, and energy applications.