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臺灣大學應用力學研究所
演 講 公 告

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主 講 人：李奕霈助理教授
臺灣大學化學工程學系

講　　題：電腦輔助機制探索與反應工程設計

主 持 人： 陳建彰教授

時　　間： 111年9月26日（星期一）下午2時20分開始

地　　點： 臺灣大學應用力學研究所國際會議廳

☆☆ 歡 迎 聽 講 ，敬 請 張 貼 ☆☆

Computer-Aided Mechanism Discovery and Reaction Engineering

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Tremendous efforts have been made for developing and improving catalysis technology to meet the growing demands of chemistry. Nevertheless, preparing novel catalysts and examining the performance of different catalysts in various conditions are often major obstacles for advancing the catalysis technology due to the tedious and costly experimental process. Computer-aided modeling, design, and optimization can facilitate the development of catalysis technology by replacing some of the many required experiments. In this presentation, I will demonstrate how one can obtain useful information from computer simulations to guide catalyst design, reactant engineering, and reaction condition optimization. Three biofuel conversion reactions occurring in zeolite catalysts including the isomerization from glucose to fructose and two renewable pathways for terephthalic acid synthesis will be used as examples for each of these topics. The prospect of combining quantum mechanical calculations with advanced machine learning techniques for efficient and robust reaction modeling will be discussed as well.