Wolfson Department of Chemical Engineering Seminar
Zoom Seminar

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Zoom Seminar

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Dr. Jianping Li

From Hangzhou Gongshu Gongda Institute of Future Technology

Title: "Molecular and Process Engineering for Sustainable Chemical Separation"

The sustainable utilization of lignocellulosic biomass requires effective recovery of bioproducts from excessive water, which is often energy-intensive. Liquid-liquid extraction is a promising low-energy separation technology, relying on molecular interactions and system-scale feasibility. For pseudoaromatic bioproducts such as 2-pyrone-4,6-dicarboxylic acid (PDC), separation can be further complicated by aggregation behavior in solution. Despite advances in separation technology and thermodynamic modeling, limited work exists to understand ions and molecular interactions during molecular aggregation, to improve property prediction of long-chain bioproduct molecules, and to assess when extraction is preferable to distillation. The objective of this talk is to address three critical questions: (1) How do molecular interactions and charge states influence the aggregation of charged, aromatic bioproducts? (2) How can molecular property prediction be made more efficient for complex solutes? (3) Under what conditions is liquid-liquid extraction more economical than distillation?

In this talk, we present a multi-scale and data-driven framework for the modeling, optimization, and analysis of separation systems to facilitate sustainable biomanufacturing and decarbonization. We first use all-atom molecular dynamics simulations and clustering-based structural analysis to examine PDC aggregation phenomena across diverse ionic solutions. Next, we present an adaptive conformer selection framework that integrates molecular dynamics with COSMO-RS (Conductor-like Screening Model for Real Solvents) calculations to improve the efficiency and accuracy of bioproduct property predictions in solvent environments. Lastly, we leveraged machine learning to identify and understand when extraction-based separation systems are more economical than conventional distillation.

Biography

Dr. Jianping Li is a Research Scientist at the Hangzhou Institute of Future Technology (officially known as the Hangzhou Gongshu Gongda Institute of Future Technology). He completed postdoctoral appointments at Argonne National Laboratory and the University of Wisconsin–Madison, while holding a joint position with the University of Chicago, as well as a visiting postdoctoral position at Princeton University. Dr. Li earned his Ph.D. in Chemical Engineering from Texas A&M University. His research focuses on the intersection of process systems engineering and molecular modeling, specifically the development of methods for process synthesis, intensification, product design, optimization, and self-assembly, with applications in energy and sustainability.