Houk-Jung Organic Colloquium

Special Organic Lecture

Bridging Chemical Knowledge and Machine Learning for Structure-Selectivity Prediction of Organic Synthesis

Abstract: As one of the key research directions in physical organic chemistry, the understanding of structure-selectivity relationship provides a rational basis for the design of molecular synthesis. Recent advancements in artificial intelligence technology offer innovative solutions for modeling and predicting these relationships. This presentation focuses on the data-driven prediction of selectivity, discussing our recent efforts to build molecular databases, design physical organic descriptors, and apply machine learning in catalyst predictions. By integrating mechanistic insights with data modeling, we demonstrate how to harness the hidden value of synthetic data for the precise design of synthetic processes. Through this report, we seek to provide the audience with a new perspective in an era where chemical and information sciences intersect.

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UCLA College | Physical Sciences Chemistry & Biochemistry

Thursday, July 18, 2024 | 4:00 PM
Mani L. Bhaumik Collaboratory - YH 4222
Dongwon Yoo Seminar & Conference Hall
& Via Zoom

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