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JACOBS SCHOOL OF ENGINEERING
NanoEngineering

UCSD NanoEngineering/Chemical Engineering

SEMINAR SERIES

Wednesday, April 17, 2024
Seminar Presentation: 11:00am – 12:00pm
SME Room 248

"The Cat-Universe: A 'Data-Theory-Methodology-Experiment' Framework to Realize Catalyst Design"

Dr. Hao Li, PhD

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Abstract: The design of solid-state materials is essential for a sustainable future. However, conventional materials search sometimes relies on the trial-and-error process from experiments. Meanwhile, the intricate structure-performance relationships of materials usually hamper the development of an effective design guideline. This talk will discuss an avenue to realize a data-driven framework for materials design combining data mining, materials theory, computational methodology development, and experiments. In particular, we will discuss i) how to reduce the complexity in catalyst design by materials theory and ii) how to develop new computational methods (i.e., package, on-the-cloud platform, model, and algorithm) to accelerate materials simulation. This talk will show the predictive power of theory in electrochemical and thermal catalysis, solid-state battery electrolytes, and hydrogen storage materials. We will also discuss the successful design of an "electron-refinery" strategy by transforming high-temperature thermal catalysis into low-temperature electrocatalysis.

Biosketch: Hao Li is an Associate Professor at the Advanced Institute for Materials Research (WPI-AIMR) of Tohoku University, Japan. He developed the "Digital Catalysis Lab (DigCat)" as the Principal Investigator in 2022. He is also the Adjunct Investigator of the ARC Centre of Excellence for Green Electrochemical Transformation of Carbon Dioxide (GETCO2), The University of Queensland, Australia. He obtained his Ph.D. degree at The University of Texas at Austin in 2019. Before his independent career, he was a postdoc researcher at Technical University of Denmark during 2020-2021, in the group of Prof. Jens K. Nørskov. Hao's research interests consist of i) development of materials and catalysis theory, ii) development of computational methodology based upon AI, and iii) design of cost-effective catalysts, batteries, and hydrogen storage materials with special emphasis on sustainable production.