



## Department of Materials Science and Engineering Seminar Series 2024

### **Theoretical Investigation on Dynamic Behavior of Bimetallic Nanocluster and Application on Propane Dehydrogenation Reaction**

**Date and time: 26<sup>th</sup> November 2024(Tuesday) 3:00-5:00 PM**

**Venue: EA-06-05**

#### **Abstract**

Understanding the dynamic behavior of bimetallic catalysts under reaction conditions is crucial for rational catalyst design, particularly for propane dehydrogenation (PDH), a vital industrial process for propylene production. While bimetallic catalysts show enhanced performance compared to their monometallic counterparts, the fundamental mechanisms underlying their dynamic structural evolution remain poorly understood. Through our comprehensive theoretical investigation combining density functional theory (DFT) and ab initio molecular dynamics (AIMD), we have uncovered significant insights into the dynamic behavior of bimetallic nanoclusters during PDH. Our systematic screening of over 90 platinum-based bimetallic nanoparticles revealed critical surface segregation phenomena governed by surface energies and formation enthalpies, leading to the identification of promising  $\text{PtM}_3$  ( $M = \text{Ni}, \text{Ti}, \text{Co}$ ) catalysts. Further investigation of PtSn nanoclusters on  $\text{Al}_2\text{O}_3$  supports demonstrated their unique liquid-like behavior at reaction temperatures, with Sn playing a dual role in both geometric and electronic modification of Pt active sites. Most notably, our study of PtSn clusters confined within MFI zeolites uncovered the crucial role of silanol nest oxygen atoms in cluster stabilization and activity enhancement, offering new perspectives for catalyst design. These findings not only advance our understanding of complex catalytic systems but also establish a new paradigm for investigating and designing next-generation PDH catalysts, with broad implications for the field of heterogeneous catalysis.

## **Biography**

Tang Yaxin received her B.Eng. degree in Materials Science and Engineering from the Southern University of Science and Technology (SUSTech) in 2018 and M.Sc. degree from Harbin Institute of Technology (HIT). She is currently a Ph.D. candidate in the Department of MSE under the supervision of Asst. Prof. He Qian. Her research focuses on understanding the dynamic behavior of bimetallic catalysts during propane dehydrogenation reactions through theoretical investigation.

**Please join us!**

HOST: Prof Ding Jun