UC San Diego
JACOBS SCHOOL OF ENGINEERING
NanoEngineering

UCSD NANO & CHEMICAL ENGINEERING
SPECIAL SEMINAR
February 15th 2023
Seminar Presentation: 9:30am – 10:30am
SME Room 248

"Short- and Long-Range Chemical Interaction in Cluster

And Condensed Phase"

Wan-Lu Li, PhD

Postdoc
UC Berkeley

Abstract: Chemical interaction is ubiquitous in daily life and can be served as an effective key to addressing different properties, but it cannot be directly detected experimentally. Computational chemistry is therefore a powerful and indispensable tool to analyze interactions along a length-scale and time-scale. In my talk, I will present computational challenges and my research progress in short-range and long-range chemical interactions that contribute to illustrating the geometrical stability, catalytic ability, and design strategies in both cluster and solid phases.

Educational Development and Training: In the past few decades, computational resources have become more powerful every year and methodology development has led to much more efficient techniques through parallelization of the calculations and the advent of density functional theory. Combined experimental/computational studies generally give a broader perspective of a chemical problem and look into it from different angles and perspectives than stand-alone experimental studies. However, although many experimentally based groups are starting to use computational chemistry methods, almost on a routine basis, nowadays there are some serious caveats with the methods and techniques and often these computational studies cannot be done through "black-box"-procedures but require expert supervision. To address the existing challenges in the area of computational chemistry, I will present my research progress on the chemical interaction-property relationship applied in both molecular and condensed phases, by leveraging or developing efficient computational tools in short- and long-range interactions, aiding understanding of the inherent stability of a system and providing design ideas of new catalyst and materials with desirable properties..

Biosketch: Dr. Wanlu Li is now a postdoc at UC Berkeley in Prof. Teresa Head-Gordon's group and is affiliated with Lawrence Berkeley National Laboratory. She obtained her PhD degree at Tsinghua University with Prof. Jun Li. Till now, she has published over 65 scientific papers among which more than 40 as the first author, and has received almost 1900 citations, the H-index is 26. She obtained the American Chemical Society Physical Chemistry Young Investigator Award in 2021, of which only 4-6 postdocs are awarded in the US each year. During her PhD research at Tsinghua University, she received National Awards in China five times, which is the highest-recognized award for a student, and was honored with "Lu Jia Xi" Fellowship for Outstanding Graduate Students, where only 20 graduate students can be awarded among all areas.