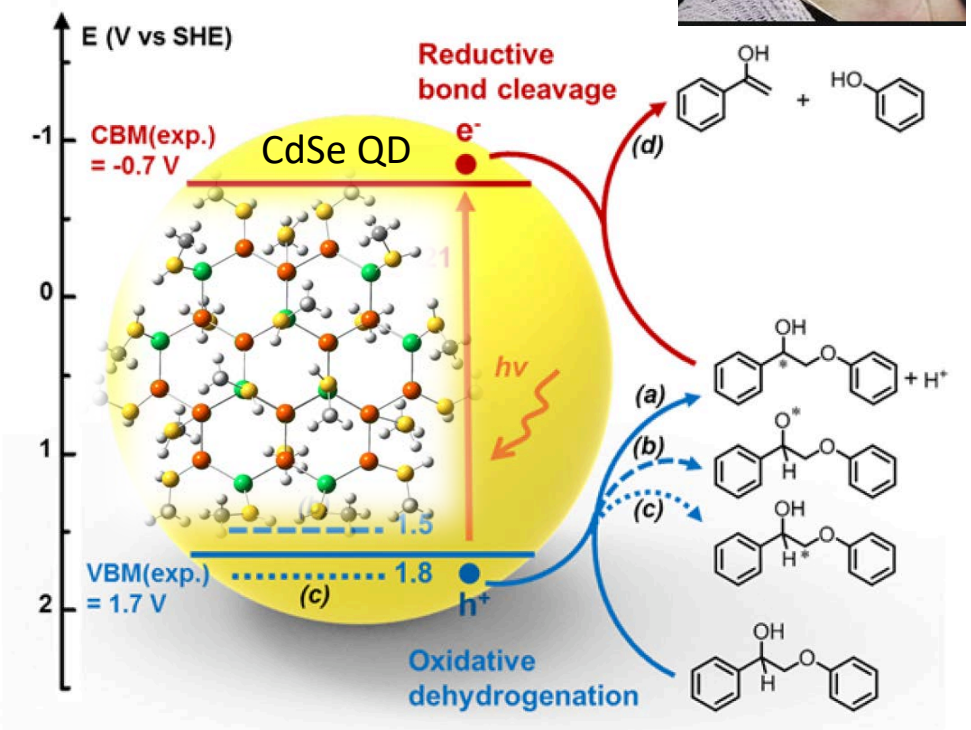
NDSU NORTH DAKOTA STATE UNIVERSITY

Modeling of Quantum Dots for Photo-Catalysis of Biomass Valorization (*Faculty Mentor:* Svetlana Kilina)

Catalytic valorization of lignin, which is potentially the largest source of renewable aromatics, represents the most attractive but challenging topic in biomass conversion. It was recently shown that CdS Quantum Dots (QD) efficiently catalyze the selective cleavage of β-O-4 bonds, the most abundant linkage in lignin through photo-redox mechanism based on a Cα radical intermediate. However, mechanism of controlling this reaction via QD engineering is unclear. In our group, we will use quantum chemistry calculations to provide important insights into mechanisms of this photo-driven reaction and the effect of the QD composition, size, and surface ligands on the photocatalytic properties governing such mechanisms.

The REU students will be trained in quantum chemistry calculations of nanostructures with complicated surface chemistry and interfaces. By the end of this research experience, students will learn how to

- use Unix operation system and run calculations at HPC clusters
- use common quantum chemistry software, such as Gaussian-16
- construct geometries and analyze calculated data
- model optical properties of nanostructures
- understand the main concepts and principles of molecular design
- perform computational studies in a tight collaboration with experimentalists



Cleavage of β-O-4 bond in the Cα radical intermediate