Nebraska Engineering

FACULTY CANDIDATE SEMINAR

University of Nebraska-Lincoln
Department of Chemical and Biomolecular Engineering

Computational and Simulation Approach on Well-Designed Materials for Energy/Environment/Catalysis Applications

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3:30-4:45 P.M.

Othmer Hall, Room 205

**Refreshments provided*

Abstract

The world's dependence on fossil fuels has led to the need for alternate sources of energy as supplies dwindle, as well as a growing need to remove harmful compounds from the air. Hydrogen energy and lithium-ion batteries are promising candidates for supplanting fossil fuels for automobile applications while novel adsorbents like metal-organic frameworks (MOFs) are promising materials for removing harmful gases. To date, my researches have been concerned with both aspects of the fossil fuel problem. Regarding hydrogen energy, my researches are focused on understanding the thermodynamics of metal hydride reactions for hydrogen storage applications. Specifically, the goal is to screen thermodynamically promising metal hydride reactions from a full database of metal hydride mixtures using first-principles calculations. The large-scale screening approach ultimately provides a number of promising single-step or multi-step metal hydride reactions. On the other hand, my research focus in the field of the lithium-ion batteries is on fundamentally understanding the redox chemistry of promising electrode materials which would directly affect the battery capacity. My researches on MOFs are related to investigating promising MOFs for the removal and separation of harmful gases. Quantum mechanical methods are used to screen and assess functional groups that would be incorporated into MOF ligands to preferentially adsorb harmful gases under humid conditions. Inspired by the research background, my future researches will be focused on developing a new paradigm which would allow us to efficiently produce and store alternative energy sources. The fundamental goal is to identify promising candidates with the fast reaction kinetics in the three main research fields: Photocatalytic carbon dioxide reduction, ionic diffusivity in the lithium-ion batteries, and metal hydride reactions. The large-scale screening approach combined with the quantum mechanical method and molecular simulations will be introduced to achieve the research goal.