USC Viterbi School of Engineering

MORK FAMILY DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE

Graduate Seminar

Presents

Using High Throughput Computation to Accelerate Development of Materials for Scalable Energy Technologies

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Abstract

Computational modeling of materials can be a powerful complement to experimental methods when models with useful levels of predictive ability can be deployed more rapidly than experiments. Achieving this goal involves judicious choices about the level of modeling that is used and the key physical properties of the materials of interest that control performance in practical applications. I will discuss two examples of using high throughput computations to identify new materials for scalable energy applications: the use of metal-organic frameworks in membranes and gas storage and the selection of metal hydrides for high temperature nuclear applications. These examples highlight the challenges of generating sufficiently comprehensive material libraries and the potential advantages and difficulties of using computational methods to examine large libraries of materials.

Wednesday, October 14, 2015
12:30 pm, HED Room 116
The scientific community is cordially invited.