



Department of Chemical Engineering presents

Professor Christopher E. Wilmer



Assistant Professor
Department of Chemical & Petroleum Engineering
University of Pittsburgh
November 8, 2017
Goergen Hall 101 @ 3:25pm

"Finding Truth in Fiction: Efficiently Discovering Physical Structure-Property Relationships By Screening Unphysical Porous Materials"

The range of physically accessible physical adsorption (i.e., physisorption) behavior in porous materials is not yet well understood. This lack of understanding has implications on our knowledge of the theoretical efficiency limits on important adsorption-related processes, such as post-combustion carbon capture. In this talk we will use classical molecular modeling to simulate adsorption of various gases in unphysical pseudomaterials," which are just random periodic arrangements Lennard-Jones (LJ) sphere systems. Importantly, within the class of pseudomaterials are all of the real materials. Therefore, by determining the limits of adsorption in pseudomaterials we necessarily also determine the limiting behavior of real materials. In this talk we will describe the methodology developed to explore this high-dimensional phase space and some results.