Physical Chemistry Seminar

Tuesday, October 15, 2013 | **11:00 am** | **Room 1315 Chemistry Building**

Accelerating Technologies for CO_2 Capture Using Computational Screening of Nanoporous Crystals

Professor David Sholl

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Host: Professor JR Schmidt

A common issue in developing nanoporous materials for specific applications is the need to choose materials with the best performance from very large numbers of candidate materials. I will describe how computational modeling can be used to accelerate efforts to address this issue. A key to achieving this goal is to use a staged approach in which increasing levels of physical detail are included as the number of materials considered is reduced. The examples discussed will focus on developing crystalline nanoporous materials as components in gas separation membranes. For this application, initial calculations are performed based on geometric principles to predict which materials will have favorable selective adsorption and transport properties for the gases of interest. Examples will include screening of > 250,000 hypothetical silica zeolite structures and complementary efforts involving thousands of metal-organic frameworks (MOFs). Once materials with promise have been identified with these geometric methods, more detailed models are required to further refine our predictions. Examples will be discussed of combining quantum chemistry and molecular modeling calculations to give high resolution predictions for adsorption and diffusion selectivity in hundreds of MOFs. Although our efforts are primarily aimed towards developing membrane applications, our calculations also give insight into applications of MOFs as highly selective adsorbents. A significant risk in performing computational materials screening is that insufficient attention is paid to the multiple factors that determine the true viability of a material in practical applications. For each factor, it is vital to take the approach that is the most time efficient. This concept will be illustrated with results from a joint modeling and experimental program in which we are developing polymer/MOF composite membranes for carbon dioxide capture from coal-fired power plants. In this work, we use experiments to probe the stability of MOFs with respect to critical flue gas contaminants and high throughput experiments to measure adsorption and diffusion properties in materials identified from our initial computational screening. Preliminary results from our efforts to fabricate polymer/MOF composite membranes in realizations suitable for scale up to the massive scale required for flue gas capture will also be presented.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335