UW Chemical Engineering

Spring 2012 Seminar Series

Computational Carbon Capture

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Date: Monday, April 2, 2012

Time: 4:00 p.m. - 5:00 p.m.

Place: PAA A110

One of the main bottlenecks to deploying large-scale carbon dioxide capture and storage (CCS) in power plants is the energy required to separate the CO2 from flue gas. For example, near-term CCS technology applied to coal-fired power plants is projected to reduce the net output of the plant by some 30% and to increase the cost of electricity by 60-80%. Developing capture materials and processes that reduce the parasitic energy imposed by CCS is therefore an important area of research. We have developed a computational approach to rank adsorbents for their performance in Carbon Capture. This ranking is based on the parasitic load a separation using this material would have on a power plant. We show how molecular simulations can be used to efficiently calculate all the required thermodynamic data. Using this analysis, we have screened hundreds of thousands of zeolite and ZIF structures and identified many different structures that have the potential to reduce the parasitic energy of CCS by 30-40% compared to near-term technologies.