# UW Chemical Engineering

***Fall 2013 Seminar Series***

**Date:** Monday, October 14
**Time:** 4:00 - 5:00 p.m.
**Place:** PAA A118
**Topic:** *Carbon Capture using Adsorption and Membrane Processes*

**Jennifer Wilcox**
Professor, Energy Resources Engineering
Stanford University

## Biography

Jennifer Wilcox has been an Assistant Professor in the Department of Energy Resources Engineering at Stanford University since 2008. Her Ph.D. in Chemical Engineering in 2004 is from the University of Arizona, and her B.A. in Mathematics in 1998 is from Wellesley College. She received the 2007 ARO Young Investigator Award (Membrane Design for Optimal Hydrogen Separation), the 2006 ACS PRF Young Investigator Award (Heterogeneous Kinetics of Mercury in Combustion Flue Gas), and the 2005 NSF CAREER Award (Arsenic and Selenium Speciation in Combustion Flue Gas). Within her research group, she focuses on trace metal and $CO_2$ capture. Her research involves the coupling of theory to experiment to test newly-designed materials for sorbent or catalytic potential. She is the author of the first textbook on Carbon Capture, recently published in March 2012.

## Abstract

The scale by which $CO_2$ must be mitigated worldwide dwarfs the existing chemical industry, making utilization of $CO_2$ as a chemical feedstock a minor component of the portfolio of mitigation options. Carbon capture and storage is one strategy that could potentially mitigate gigatons of $CO_2$ emissions per year, provided the storage potential exists. Strategies based upon adsorption and catalytic membrane separation processes will be discussed. In particular, carbon-based micro and mesoporous materials for selective $CO_2$ capture and dense metallic membrane materials for selective $N_2$ separation from $CO_2$ will be of focus.

Modeling and simulation play an important role in the construction of realistic pore structures and also aid in understanding adsorption-desorption mechanisms. Density functional theory calculations have been performed to investigate the electronic properties of graphitic surfaces and charge analyses have been carried out to generate partial charge distributions of graphitic surfaces with surface-embedded functional groups. Grand canonical Monte Carlo is used to simulate the adsorption processes and different potential models for the $CO_2$ molecule are adopted to calculate the interactions between fluid molecules and between fluid molecules and pore walls. The effects of various pore sizes, potential models, temperatures, and surface heterogeneity will be discussed.

In addition to adsorption investigations, metallic membrane materials for selective $N_2$ separation for carbon capture are also under investigation. This work involves the adsorption, dissociation, and sub-surface diffusion of $N_2$ in Group V-based metals, including vanadium, niobium, and their alloys with ruthenium. The electronic structure of the metal can be tuned based upon alloying, thereby enhancing $N_2$ permeability. Experimental $N_2$ flux measurements are underway to test the theoretical predictions and preliminary results will be presented.