Chemistry and Molecular Biology Department
Seminar
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"Minimizing Environmental Impacts of Coal-based Energy Generation"

Dr. Jennifer Wilcox
Assistant Professor, Department of Energy Resources Engineering, Stanford University

Abstract

With the United States generating over half of its electricity from coal combustion, and with more than five hundred 500 megawatt, coal-fired power plants existing in the United States with an average age of 35 years, coal as a significant future energy source is inevitable. To minimize the environmental impacts of coal burning and to increase the sustainability of this abundant resource, advancing "clean coal" technologies is imperative. Worldwide, the primary power-generating coal-based technology is pulverized coal combustion. Within the past two decades there have been great strides in reducing harmful emissions associated with this technology, specifically involving the reduction of pollutants such as SO_x, NO_x, particulates, and mercury. In addition to the release of these pollutants, coal burning is the largest contributor to global CO_2 emissions from energy generation; therefore, in the production of new coal-based power-generating technologies, e.g., coal gasification, minimizing these environmental hazards must be taken into consideration.

In particular, a complete homogeneous kinetic model for mercury oxidation generated from *ab initio*-based rate constant data was developed and validated through focused experiments which included simulating flue gases through methane combustion. It has been concluded that the majority of mercury oxidation occurs heterogeneously, likely via unburned carbon. Knowledge of mercury's oxidation pathway has also led to the design of a nanostructured sorbent material for its subsequent capture. This new palladium-based material that was generated in our lab has been computationally designed using density functional theory-based energetics obtained from VASP (Vienna *ab initio* Simulation Package), which allow for mercury capture at the higher temperatures, 260-315 ºC, typical of coal gasification applications. We discovered that the addition of small amounts of gold, i.e., 12.5%, created more favorable hcp three-fold palladium adsorption sites for mercury binding. In contrast to this unique application, palladium-based materials have been modeled for their solubility, diffusivity, and subsequent permeability of hydrogen to be applied to separation applications. The addition of a membrane reactor utilizing this technology will be useful for the separation of CO_2 in a syngas stream from coal gasification processes. In total, the overall motivation behind these efforts has been to minimize the environmental impacts of energy generation from coal-based technologies.

Bio: Dr. Jennifer Wilcox received a Bachelor's degree in Mathematics from Wellesley College in 1998 and received a Master's degree in Physical Chemistry and a Ph.D. in Chemical Engineering from the University of Arizona in 2004. She joined Worcester Polytechnic Institute as an assistant professor in July 2004 and has recently relocated to the Department of Energy Resources Engineering at Stanford University. She has received the NSF Career award for her work in trace element speciation in combustion flue gases and has received the Army Young Investigator award for her work in hydrogen separation with Pd-based membranes.