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CSU PHYSICS COLLOQUIUM

Adsorption Kinetics of Gases on Carbon Surfaces

Speaker: Maria Mercedes Calbi

Affiliation: Department of Physics and Astronomy, University of Denver

Colorado State University

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Refreshments at 3:45 PM

Location: 120 Engineering (Hammond Auditorium)

Abstract

Adsorption phenomena on surfaces have been extensively investigated based on the presence of thermodynamic equilibrium between the external gas in contact with the surface and the adsorbed film. In nanoporous structures, however, the actual observation of expected equilibrium properties (the total gas uptake, for example) may strongly depend on how and how fast that equilibrium is reached, generally referred to as adsorption kinetics. Processes such as diffusion into the interior of the structure and particle transfer from one group of sites to another may encounter different energy barriers that limit and/or significantly delay access to the adsorption sites. While this may be detrimental for the storage performance of the nanostructure, it can alternatively be exploited as means for separating different gases from a mixture. Gas separation devices are widely used, for example, for O₂ production out of air, CO₂ removal from flue emissions and for biogas upgrading.

We present here a series of results concerning the kinetics of adsorption of different gases and mixtures on different regions of a carbon nanotube bundle. Since these nanostructures have several kinds of adsorbing surfaces (including pores and inhomogeneous external surfaces) our results are also relevant to many other adsorbents that typically have only one type of these surfaces. By implementing a Kinetic Monte Carlo algorithm to follow the time evolution of the gas uptake we are able to explore an interesting variety of kinetic phenomena, identifying the elemental processes responsible for such behavior. As a result, we have provided useful insight on long standing controversies on the adsorption behavior of these structures as well as direct explanation of several adsorption kinetics experiments.

Biographical Sketch

Born and raised in Argentina, Prof. Calbi earned her PhD degree in physics at the University of Buenos Aires in 2000. She then completed her training in condensed matter physics at the Pennsylvania State University where she made her first contributions in the theory of gas adsorption on solid surfaces. In 2003, she joined the Physics Department at SIUC, and later on she moved to University of Denver where she has been Associate Professor in the Physics & Astronomy department for the last five years.

One of her main interests lies on determining the ability of a variety of nanostructures to act as adsorbents by developing models and methods that can provide a basic understanding of the adsorption processes and phenomena (equilibrium and kinetics) in nanoporous materials. From a practical perspective, the goal is to provide a rational basis for assessing the performance of a nanostructure for specific adsorption applications that can be used, at the same time, to guide the design of new materials for such uses.

Prof. Calbi's research projects have been continuously funded by external agencies since 2005 and are currently supported by the National Science Foundation. She is the recipient of a CAREER award from that agency, and was also honored in 2010 with the "Presidential Early Career Award for Scientists and Engineers" (PECASE).