Skilled at Working Small

by Tim Crosby

Understanding the mechanics by which molecules bind to tiny nanotube bundles could have big ramifications for energy storage, air purification, environmental remediation, and other challenges.

One of SIUC's latest faculty to win a coveted National Science Foundation CAREER award is using nanotechnology to make advances in areas related to energy storage and other applications.

María de las Mercedes Calbi, assistant professor of physics, received a five-year, $400,000 grant to develop theoretical models and methods aimed at understanding how molecules and atoms gain access and bind to carbon nanotube bundles.

CAREER awards, which are highly competitive, aim to establish promising junior researchers by providing long-term funding for their work. The grants also integrate student outreach and education.

Calbi's work has great potential for areas such as gas separation, purification, and storage. Although atom and molecule adsorption has been used for some time in areas such as gas separation, Calbi's work moves the concept forward by focusing on how carbon nanotube bundles behave in this arena.

The bundles are extremely tiny collections (a nanometer is one billionth of a meter) of long, hollow tubes that form spontaneously under given conditions. Because of their shapes and porous nature, the structures provide several different types of surfaces as bonding points for atoms and molecules, and thus a high amount of total bonding area.

The atoms and molecules can attach themselves inside a nanotube or along the valley-like areas that run along the outside of the tubes, for instance. The structures also contain interstitial pores between the tubes, which provide additional potential bonding points.

Such nanotube structures are promising materials for separation and membrane applications. When they're fully understood, one possible use might involve efficient hydrogen storage methods, which could open a variety of environmentally sound technologies. Other possible applications include air purification systems and environmental remediation.

Among other things, Calbi wants to know how to ensure the strongest possible bond between the gas and the nanotube bundles. She also wants to study how quickly certain atoms and molecules can gain access to and bond with a surface, a topic known as adsorption kinetics.

Part of Calbi's project will look at the relationship between the size of a pore in relation to the size of an atom or molecule and how that affects bonding strength. Generally, the closer the size match, the stronger the bond—but this also makes access more restrictive. Calbi will examine how this trait plays into the overall question of adsorption.

Using different atoms and molecules under various conditions, she and her students also will look for efficient combinations that balance the time it takes for adsorption against the energy required to do so.

Although she'll focus on nanotube bundles to extract this knowledge, Calbi's goal is to discover the basic principles that could be used to understand such processes in other nanomaterials, or even to design nanostructures with specific applications.

Because of its nanoscale nature, Calbi's work will delve into the world of quantum mechanics, which operates under an entirely different set of laws than classical physics.

"Much of it is really unknown," Calbi says. "When you have diffusion of molecules in restricted spaces, such as inside a nanotube, the molecules can behave in a very different way."

Calbi's work will be done mostly with theoretical models and computer simulations. However, she'll also work closely with Aldo Migone, professor and chair of the physics department. He'll test various concepts in his laboratory, confirming or disproving the various theories and models Calbi's team advances.

Three graduate students and one undergraduate are working with Calbi on the project. Junior Jared Burde recently won third place at SIUC's Undergraduate Research Forum for a poster describing his part of the work. Calbi also plans a new physics course on surface science at the nanoscale, which will emphasize using computers to model processes that occur in such a small realm.

"It will teach students how to use a computer as a tool for doing physics research," she says.

For more information: Dr. Mercedes Calbi, Dept. of Physics, mcalbi@physics.siu.edu. Assistant professor of chemistry Punit Kohli, whose work in nanotechnology was featured in our fall 2006 issue, also received a CAREER award recently; *see p. 24.*

Left: Mercedes Calbi gives a rough demonstration of binding sites for gas molecules on nanotube bundles. Right, top: Master's student Seyoum Tsige and Calbi go over some calculations. Right, bottom: Material about a particular adsorption model.