Neutron scattering provides window into surface interactions

January 17 2012

To better understand the fundamental behavior of molecules at surfaces, researchers at the U.S. Department of Energy's Oak Ridge National Laboratory are combining the powers of neutron scattering with chemical analysis.

Scientists have a fundamental interest in how molecules behave at solid surfaces because surface interactions influence chemistry, such as in materials for catalysis, drug delivery and carbon sequestration. Understanding these interactions allows researchers to tailor materials for a specific desirable outcome.

Michelle Kidder and A.C. Buchanan, physical organic chemists, and Ken Herwig, neutron scattering scientist, used neutron scattering to study the physical motion of a chemically attached organic molecule inside a silica nanopore, MCM41.

"There is a connection between a molecule's dynamic behavior or motion to its surroundings." Herwig said. "In particular, restricting the ability of a molecule to freely move by confining it to a small volume dramatically affects both the range and character of its movement. We are trying to gain insight into the connection between the changes in molecular motion and the changes in chemistry that occur when molecules are attached to a solid surface."

Herwig used neutron scattering to gain a unique perspective into molecular motion because neutrons are sensitive to the hydrogen atoms,

which are present in many molecules that researchers are interested in. Additionally, neutron scattering simultaneously tells researchers how rapid the motion is and what type of motion they are observing on the atomic and nanoscale.

If scientists understand how pore size affects surface interactions, they can modify pore size to change a chemical product outcome.

To study surface interactions, Kidder synthesized both the organic molecules and MCM41 of different pore sizes, then chemically attached the molecules to the silica pore surface, which forms an organic-inorganic hybrid material. This hybrid material is used in studies to understand chemical decomposition pathways, where surface interactions were presumed to play a role.

"We are interested in understanding the thermo decomposition of molecules similar to those found in biomass resources," Kidder said. "What we have seen is that there are many local environmental factors that influence chemical reactivity and products, and one of those large influences occurs when a molecule is confined to a pore wall, where even the pore size has a large impact on reactivity."

More information: These findings were published in a paper, "The Dynamics of 1, 3 diphenylpropane Tethered to the Interior Pore Surfaces of MCM-41," which appeared in *J Physical Chemistry C.*

Provided by Oak Ridge National Laboratory