Energy Solutions from Catalysis Research

Catalysis research is playing a key role in developing solutions for energy needs, environmental protection, and the problem of global warming.

How water molecules move at the interface with solids is one of the more urgent questions in current research into catalytic materials. Using a combination of neutron scattering and molecular dynamics simulations, researchers at SNS were able to probe interfacial water dynamics on a time scale from a nanosecond (1 billionth of a second) to a picosecond (1 trillionth of a second). In the process, they gained a fundamentally new understanding of how water engages a surface at varying temperatures. Water is a key element in many catalytic reactions, and the ultimate goal is to develop new catalytic and catalyst-support nanomaterials. Those nanomaterials can then be used as catalysts for chemical production processes in various industries.

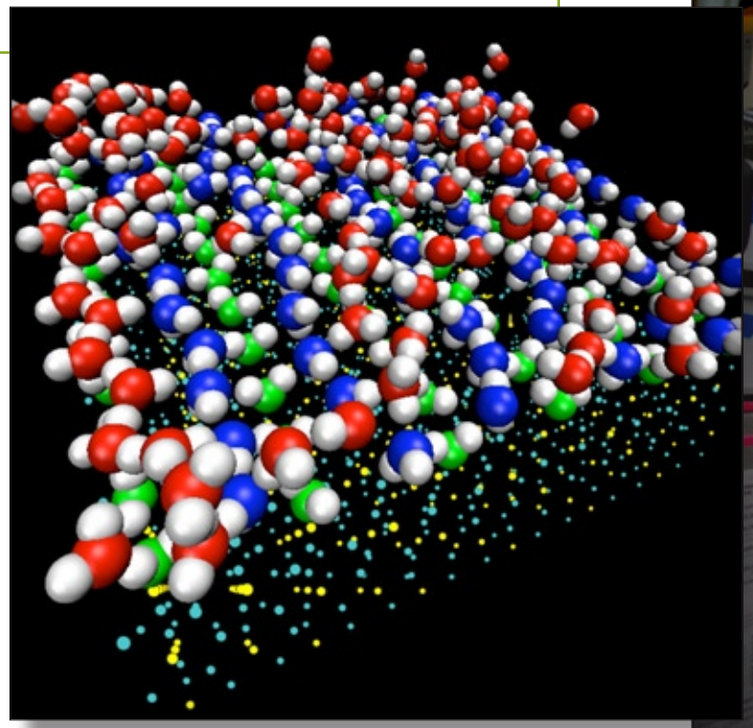
"Catalysis is important for energy and the environment because virtually all chemical production processes are assisted by catalysts of some kind," says Eugene Mamontov, lead instrument scientist for the SNS Backscattering Spectrometer (BASIS). "In particular, oxide nano-powders, rutile among them, are commonly used in various applications as catalysts, catalyst supports, or both." In their research, the team studied how water molecules move on the surface of rutile and how the water dynamics were affected by changes in temperature. They used BASIS, which measures subtle changes in the energy of neutrons that are scattered by the sample (in this case, the mobile water molecules on the rutile nanopowder surface).

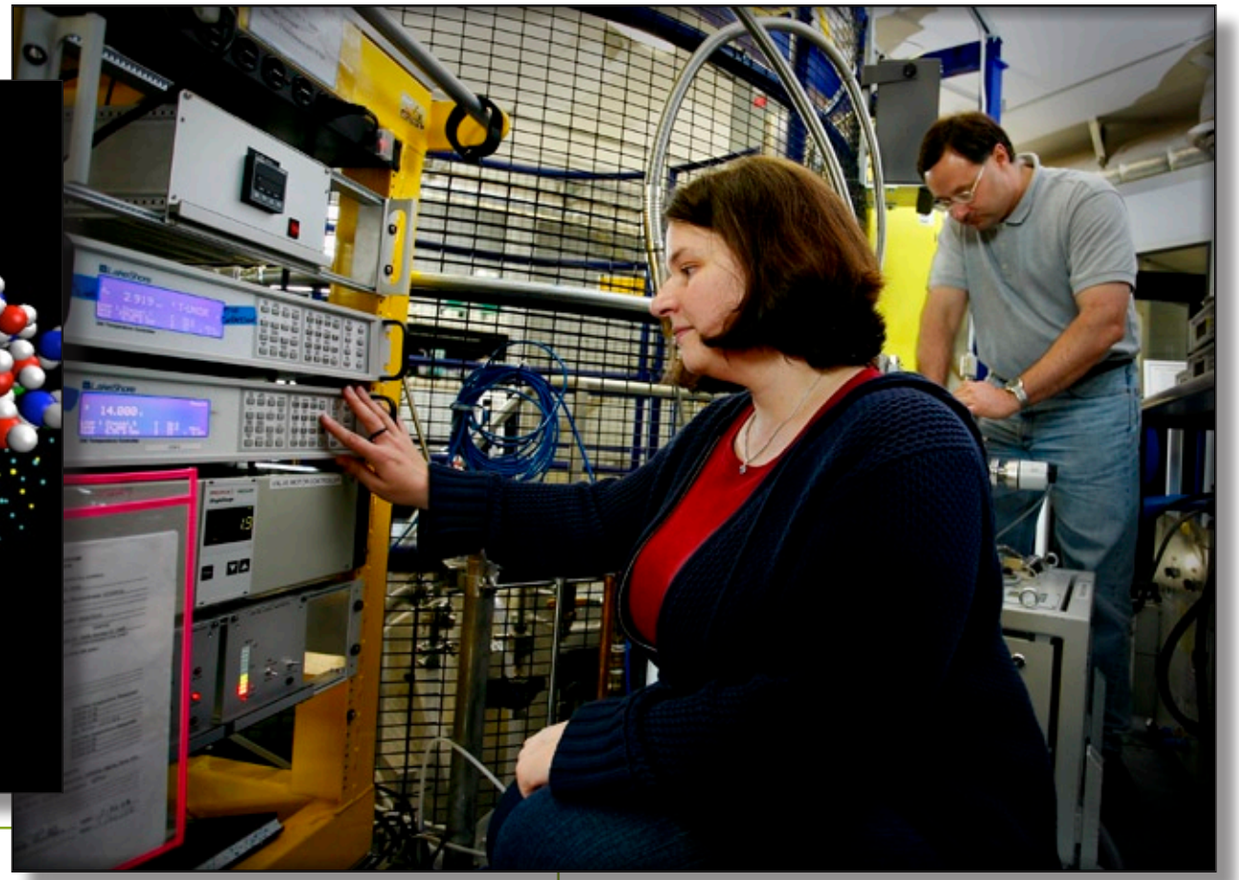
"Nanoscale Complexity at the Mineral/Water Interface" is a big-umbrella project, funded by the Division of Chemical Sciences, Geosciences and Biosciences, which is part of the DOE Office of Basic Energy Sciences. Led by principal investigator David Wesolowski of the ORNL Chemical Sciences Division (CSD), it has a number of participants who combine their expertise in several fields to attain a comprehensive understanding of interfaces. Part of their recent research entailed experiments with water on rutile—a form of the highly refractive mineral compound titanium oxide. The work engaged participants Wesolowski, Mamontov, Lukas Vlcek (Vanderbilt University), Peter Cummings (Vanderbilt and the ORNL Center for Nanophase Materials Sciences), Jorgen Rosenqvist (CSD), Wei Wang of the ORNL Environmental Sciences Division, Dave Cole (CSD), and more than a dozen other researchers. "The scope of this project is very broad, for we are developing a fundamental understanding of the phenomena which occur at water-mineral interfaces," Mamontov said.

"What makes this spectrometer unique is that it utilizes a very high intensity neutron beam; but even more so, its combination of high-energy resolution and wide dynamic range is unprecedented," Mamontov said. "This enabled us to probe the dynamics on a time scale from 1 nanosecond (1 billionth of a second) to 1 picosecond (1 trillionth of a second). In particular, we were able to probe the dynamics of surface water on the rutile sample down to 195 K (-109°F), even though the motions become very slow at such a low temperature." To better understand their results, neutron scientists then used the Computing Center at Vanderbilt University, where the team used molecular dynamics simulations to "label" and track individual water molecules and their motions.

The results of the water on the titanium oxide surface experiment gave the researchers a new understanding of the dynamics in great detail, Mamontov said. "Under ambient conditions, the surface of any hydrophilic material (materials which attract water, such as oxides) is covered by a thin layer of water ad-

Catalysis research revealed the dynamics of surface water on catalytically active nanomaterials.





Michaela Zamponi (left) and Eugene Mamontov (right), instrument scientists for BASIS.

sorbed from the atmosphere. If you expose the material to open air for a short time, the surface will be covered by adsorbed water. The coverage is thin—only about 2 or 3 molecular layers of water—but these molecules exert great influence on the surface properties of the material, especially in the case of nanomaterials, such as nano-powder oxides, simply because the surface area is so large."

"It's the fact that hydration water is so ubiquitous on the surface of hydrophilic materials that gives broad significance to this research. We found that this thin layer of adsorbed surface water (also called hydration water) does not really freeze; even at temperatures as low as 195 K, it shows some mobility. How this water moves depends on the hydration level (for example, whether we have two layers, or three layers of water). The research has great potential for catalytic and catalyst-support nanomaterials." The team will now conduct further experiments, using different materials hydrated with water and exploring the dynamics of different hydration levels of water on the materials, Mamontov said. "This is an ongoing project and will span at least several years."

For more information see:

E. Mamontov, D. J. Wesolowski, L. Vlcek, P. T. Cummings, J. Rosenqvist, W. Wang, and D. R. Cole, Dynamics of hydration water on rutile studied by backscattering neutron spectroscopy and molecular dynamics simulations, J. of Phys. Chem. C 112, p. 12334, 2008.

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