William R. Wiley
EMSL In Brief
Environmental Molecular Sciences Laboratory

900-MHz NMR Enables Novel Catalysis Studies

The ability to tailor catalysts one atom at a time is a step closer to reality, in part, because of the 900-MHz nuclear magnetic resonance spectrometer (NMR) at the Environmental Molecular Sciences Laboratory (EMSL). Researchers from the Institute for Interfacial Catalysis (IIC) at the Pacific Northwest National Laboratory (PNNL) have used the 900-MHz NMR to generate the highest resolution spectra ever obtained of a common catalyst support and observed, for the first time, how the support interacts with a catalyst at the atomic scale.

EMSL's 900-MHz NMR is enabling catalysis studies never before possible.

To really understand catalysts, they must be studied in molecular and atomic detail. Peering closely, the IIC team, led by PNNL's Chuck Peden, characterized a model system of the common γ-alumina support, γ-Al_2O_3, and the catalyst, barium oxide (BaO). γ-alumina materials serve as a support material for many catalysts, including BaO. Because BaO absorbs NO_x – a family of vehicle emissions products – the model system is a promising combination for emissions control.

Despite the importance of γ-alumina materials, technology has previously not allowed detailed studies of them. Peden said, "The chemical properties of γ-alumina compounds are such that using traditional surface structure techniques to study them is not feasible. EMSL's 900-MHz NMR allowed us to perform studies not possible before."

Using the 900-MHz NMR, Peden and his team obtained the highest resolution NMR spectrum of γ-Al_2O_3 known to date. They also observed, for the first time, where and how a catalytically active phase (BaO) interacts with the surface of an aluminum oxide as the catalyst is being synthesized.

The team's data suggest that five-fold coordinated Al^{3+} ions form a nucleation site on the surface of γ-Al_2O_3 on which BaO molecules collect. In fact, changes in the NMR spectra obtained using varying levels of BaO showed a nearly mole-per-mole correlation between the penta-coordinated Al^{3+} ions consumed and catalyst deposited.

Peden presented his findings, recently published in the *Journal of Catalysis*, at the AVS 54th International Symposium in Seattle.

In future studies, the team will examine the interaction of γ-Al_2O_3 with other metal and metal-oxide particles of catalytic interest to determine if penta-coordinated Al^{3+} ions are nucleation sites for other catalysts.

For more information, contact Mary Ann Showalter (509-376-5751).