

Dynamics of Surface Water in ZrO_2 Studied by Quasielastic Neutron Scattering*

Eugene Mamontov (NIST/CHRNS) **DMR-0086210**

High surface area oxides have found wide technological applications in catalysis. Under ambient conditions, adsorbed water exerts a great influence on the surface properties of these nanoparticulate systems, which have specific surface area of tens or hundreds meters squared per gram.

CHRNS instrumentation was used to elucidate the dynamic behavior of water on the surface of ZrO_2 . This study showed that:

- The oxide surface is terminated with hydroxyl groups and that there are two water layers on top of the surface hydroxyl layer;
- The top water layer has a translational time constant that is considerably longer than for bulk water while the rotational time constant is only slightly larger than for bulk water; and
- The average jump distance for the molecules in the top layer (about 4.3 Å) is the same as the average distance between the surface hydroxyl groups.

*E. Mamontov, *J. Chem. Phys.*, in press.

