Ninth Conference on Computational Research on Materials
Morgantown, West Virginia
May 19–21, 1999

A Computational Investigation of Unusual Chemistry of Catalytic Aluminas*

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We report first-principles calculations that led to the discovery that gamma-alumina has a remarkable property. It behaves as a sponge, in that it can store and release water, but in a unique, ``reactive'' way. When a water molecule arrives at the surface it breaks up, H enters the bulk, and O stays at the surface. Al atoms counter-migrate from the bulk to the surface where they combine with the new O atoms and extend the bulk. The reverse process is also possible: H comes out from the bulk and combines with surface O to evolve as water while surface Al atoms counter-migrate into the bulk. We will show that this unusual chemistry is a natural consequence of the fact that gamma-alumina is not a single substance, but is a sequence of hydrogen-containing forms

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*This research was sponsored by the Division of Materials Sciences, U. S. Department of Energy under contract No. DE-AC05-96OR22464 with Lockheed Martin Energy Research Corp.

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