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How Gamma-Alumina Surfaces Breathe Water and Eat Aluminum*

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Gamma-alumina, one of the so-called transition aluminas, is a hugely important industrial material, but its structure and even composition have been debated for decades. We have carried out computational studies on gamma-alumina and found that, in-fact, gamma-alumina exists over a range of compositions, all based on the same spinel structure, but with varying hydrogen content. Predictions, based on these structures, of the density profile, bulk OH vibrational frequencies, and hydrogen mobility are all in good accord with experimental results from the literature. We have further found that the mobility of the bulk hydrogen leads to very unusual surface chemistry. Understanding this surface chemistry allows us to understand some perplexing experimental results: STEM images of ultradispersed metal atoms on a gamma-alumina surface, and Al-27 surface NMR.

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