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Unusual Chemistry of Catalytic Alumina Surfaces*

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An atomic-level understanding of catalytic systems would be a very powerful tool to aid the selection of catalytic materials and optimize their properties. At present, however, there is very limited information on the atomic configurations of the active sites, their electronic structure, and activation barriers for surface and subsurface diffusion, oxidation and reduction. Without such information, atomistic mechanisms are largely a matter of speculation, and their development is mostly empirical. Here we present an atomic-scale description of the gamma-alumina surface, through a combination of Z-contrast imaging of atomic configurations and first-principles calculations. The picture that results is one of remarkable surface chemistry.

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