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## DFT Calculations for $\gamma$ -Alumina Bulk and (110) Surface

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Density functional theory calculations on  $\gamma$ -alumina bulk and the preferentially exposed (110) surface are reported. The calculations reveal that  $\gamma$ -alumina may contain hydrogen over a range of concentrations and that this hydrogen becomes mobile at elevated temperatures. Calculations of the energy barrier to hydrogen diffusion predict kinetics in excellent agreement with experiments. It is found that when the (110°C) layer of  $\gamma$ -alumina is exposed, it undergoes a massive spontaneous reconstruction. The three-coordinated Al atoms initially in the surface layer drop into vacant octahedral interstices in the next lower layer. This result explains the perplexing experimental observation that no three-coordinated Al is observed on  $\gamma$ -alumina surfaces, despite the fact that its presence should be expected based on the bulk structure. Understanding the structure of the complex gamma alumina surface is an essential first step in determining the origins of catalytic activity.

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