Oxides Surfaces and Nanoparticles: from atomic surface structure to thernodynamically stable face selective catalysis

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Oxide surfaces are an important frontier, with numerous applications in areas ranging from catalysis to oxide electronics. Despite this, our understanding of oxide surfaces is relatively primitive. There is a large body of evidence indicating that many oxide surfaces reconstruct with large unit cells, making elemental metals or semiconductors look simple. Indeed, the simplest perovskite SrTiO3 has many more reconstructions than silicon. Using techniques based upon careful collection of diffraction data coupled with detailed DFT analyses we have made substantial progress in understanding these surfaces over the last few years. For instance, we used a multi-technique solution for a series of reconstructions on the $SrTiO_3$ (110) surface as well as a large reconstruction on $SrTiO_3$ (001).

While this by itself is useful science, it is not always obvious how this translates to results of technological importance. One area where it does is heterogeneous catalysis, i.e. nanoparticles supported on these oxide surfaces. It turns out that depending upon the surface structure one has different epitaxy of the nanoparticles, and in turn difference for face-selective catalysis.

In this talk I will describe how our older work on $SrTiO_3$ surfaces [1-7] has led to the start of understanding and design of face-selective catalysis for Pt/$SrTiO_3$ [8-11]

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