

MAR14-2013-020228

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Correlating structure and function for nanoparticle catalysts

GRAEME HENKELMAN, University of Texas at Austin

Better oxygen reduction catalysts are needed to improve the efficiency and lower the cost of fuel cells. Metal nanoparticles are good candidates for new catalysts because their catalytic properties are different from bulk metals, and are sensitive to particle size, shape and composition. The electronic structure can be determined for small particles, making it possible to optimize particles for a desired reaction. Here, we calculate the electronic structure of 1 nm core/shell particles and show how the energy of electrons in the shell can tune the binding of oxygen by varying the core metal. Transition state calculations for O₂ dissociation on the nanoparticle surface show that the d-band center is a good measure of the activation and reaction energies. Two factors are found to be significant for determining the catalytic activity of small nanoparticles; charge transfer in core/shell particles and the rigidity of alloy particles.