

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**First principles studies of the oxygen reduction reaction on the Pd-Co surfaces.** SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — Fuel cells (FC) are promising means for obtaining clean energy, however Pt-based catalysts currently used in FC are too expensive for practical application. Since Pd-Co nanostructures are found to show enhanced electro-catalytic properties for the oxygen reduction reaction (ORR) on FC's cathode catalysts, we focus on these materials. We carry out density functional theory calculations using the Vienna AB initio Simulation Package (VASP) in order to investigate ORR characteristics of the  $\text{Pd}_x\text{-Co}_{1-x}$  ( $x=0.75$  &  $0.5$ ) surfaces. We have calculated the absorption energies of O and OH for different sites in the surface and use them to build a free energy diagram, which helps us to estimate the ORR rate as proposed in [1]. Since experiment suggests an alloy segregation leading to formation a single Pd layer on the surface, we have performed the calculations for this system as well. The calculation results suggest that the Pd layer on  $\text{Pd}_{0.75}\text{-Co}_{0.25}$  has the onset potential for ORR higher than that for non-segregated systems and clean Pd. We also trace these properties to calculated densities of electronic states of the materials. [1]J.K Nørskov, et al, J.Phys.Chem.B,108,17886(2004)

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Date submitted: 05 Jan 2010

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