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First principles design of the Pd/Co/Pd sandwich-like structure as a promising electrocatalyst for the oxygen reduction reaction on hydrogen fuel cell cathode SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — In the search of Pt free catalytic materials, experiments have shown an enhancement in the catalytic activity of Pd-Co alloys over Pd surfaces, comparable to the one obtained with Pt, as well as a Pd enrichment of the topmost layers. In this work we present the rational design of a new catalyst material towards the oxygen reduction reaction (ORR) consisting on Pd(111) surface sandwiched with Co as the second layer (Pd/Co/Pd). The calculated reaction free energy diagrams confirm that the proposed sandwich-like structure is highly active towards ORR. The higher catalytic activity of the Pd/Co/Pd system is traced to the change in the electronic local density of states of the Pd surface atoms. Namely the hybridization of the Pd d-states with the Co majority-spin band causes a low-energy shift of the Pd d-band. This results in a reduction of surface reactivity which is favorable for ORR. We have also studied form first principles the stability of the system and evaluated the dissolution potential of Pd in Pd/Co/Pd. The results suggest that the system will be stable in the reaction environment.

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