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First principles studies of the oxygen reduction reaction on Se-Ru nanostructures SEBASTIAN ZULUAGA, SERGEY STOLBOV, University of Central Florida — Experiments show an enhanced rate of the oxygen reduction reaction (ORR) on Se-Ru nanostructures (NS) in hydrogen fuel cell cathodes. We use first principles methods to study Ru and Se-Ru NS of approximate 1.2 nm size and shine some light on how the Se affects the O and OH adsorption, which is the bottle neck of the power delivered by the fuel cell. Experiments shows that the Se-Ru NS have a Ru core but is not clear how the Se is distributed on the surface. Our calculation shows that the Se atom adsorbs on the Ru surface with a binding energies in the range 5.7 to 7.1 eV with electronic charge transfer from the Ru atoms. Due to repulsion between negatively charged Se atoms, they tend to spread uniformly over the the Ru NS rather than form islands on its surface. We have also found that, in contrast to the flat Ru surface, the Se bond to the low coordinated Ru atoms have significant covalent component. Our calculation shows how the presence of Se atoms affects the adsorption of the ORR intermediates on the NS. In particular, we show that the electrostatic repulsion between charged Se and O or OH reduces the binding energy of the latters.

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