

Abstract Submitted
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The Se effect on the oxygen reduction reaction on the Se/Ru electro-catalysts. Insight from first principles. SERGEY STOLBOV, University of Central Florida — Rational search for new efficient low-cost electrocatalysts for oxygen reduction reaction (ORR) on the hydrogen fuel cell cathodes focuses on varying the material composition to modify the local densities of electronic states (LDOS) of the surface atoms, in order to tune the surface-adsorbate electronic state hybridization and hence binding energies of the ORR intermediates. My calculation results for the Se/Ru electrocatalysts suggest an alternative way of tuning the binding energies. The Se atoms deposited on the Ru surface are found not to change Ru LDOS noticeably, however, Se atoms are negatively charged due to ionic Se-Ru bonding. As a result, they repel electrostatically the adsorbed negatively charged O and OH intermediates, and this way reduce their binding energies. Since for the Ru case, reduction of the O and OH binding energies makes ORR energetically favorable, Se deposition dramatically improve the ORR rate on Ru. The ORR rate can thus be enhanced by changing coverage of the deposited halchogen atoms or by tuning the charge transfer to those by modifying the substrate composition.

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