

Oxygen Reduction Reaction on Pt Overlayers Deposited onto a Gold Film: Ligand, Strain, and Ensemble Effect - DTU Orbit (08/11/2017)

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We study the oxygen reduction reaction (ORR), the catalytic process occurring at the cathode in fuel cells, on Pt layers prepared by electrodeposition onto an Au substrate. Using a nominal Pt layer by layer deposition method previously proposed, imperfect layers of Pt on Au are obtained. The ORR on deposited Pt layers decreases with increasing Pt thickness. In the submonolayer region, however, the ORR activity is superior to that of bulk Pt. Using density functional theory (DFT) calculations, we correlate the observed activity trend to strain, ligand, and ensemble effects. At submonolayer coverage certain atom configurations weaken the binding energies of reaction intermediates due to a ligand and ensemble effect, thus effectively increasing the ORR activity. At higher Pt coverage the activity is governed by a strain effect, which lowers the activity by decreasing the oxidation potential of water. This study is a nice example of how the influence of strain, ligand, and ensemble effects on the ORR can be deconvoluted.

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Authors: Deng, Y. (Ekstern), Tripkovic, V. (Intern), Rossmeisl, J. (Ekstern), Arenz, M. (Ekstern)

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