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# A Theoretical Study of Oxygen Reduction Reactivity on Disordered Binary Alloy Surfaces

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## ABSTRACT

In the present paper, $Pd_xCu_{1-x}$ disordered binary alloys with promising properties for the ORR were studied. The approach suggested by Nørskov et al. was applied in order to obtain the free energies of different reaction intermediates on (111) surface of $Pd_xCu_{1-x}$ disordered binary alloys, with values of 0.80, 0.85, 0.90, and 0.95 of Pd concentration. The free-energy differences take solvation, entropic, and zero point energies into account. Subsequently, we construct the hybrid free energy diagrams (FED) by also including the activation energy barriers for different O–O bond scission steps in the ORR network. Finally, by performing a Sabatier analysis, the free energy changes and activation energy barriers for relevant steps are used to estimate the relative activity of these catalysts at cell potentials of 0 V, 0.80 V and 1.23 V.

***Keywords:*** $Pd_xCu_{1-x}$; disordered; binary.