# Oxygen activation on carbon coated iron nanoparticles; Insights into the mechanism of Fe-N-C catalysis

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This work investigates the feasibility for molecular oxygen activation and dissociation on the $sp^2$-hybidized surface of carbon in carbon-coated iron nanoparticles. The possibility to develop a non-precious metal catalyst for oxygen reduction reaction in for application in low-temperature polymer electrolyte membrane fuel cells has attracted the attention of the materials' science community. Our fundamental theoretical study is performed using density functional theory with generalized gradient approximation. The geometry and electronic structure of the carbon-coated iron nanoparticles were elucidated, revealing the nature of C-Fe binding interaction and the resulting carbon surface electronic states modification. The Fe-induced carbon catalytic activity was explained through core-shell electronic interaction within the carbon-coated iron nanoparticles. Molecular oxygen activation to superoxo and peroxo states was studied using the nudged elastic band method as shown in Figure 1. Electron transfer leading to the molecular oxygen activation was investigated in detail and assigned to the nanoparticle's core-shell properties. The effect of nitrogen doping into the carbon shell was taken into account and its influence on the particle's properties and electronic structure. Degradation mechanisms of the carbon-coated iron nanoparticles were investigated which could proceed as parasitic reactions in the course of oxygen activation. The study provides novel theoretical insights into the Fe-C-N catalyst's functions.

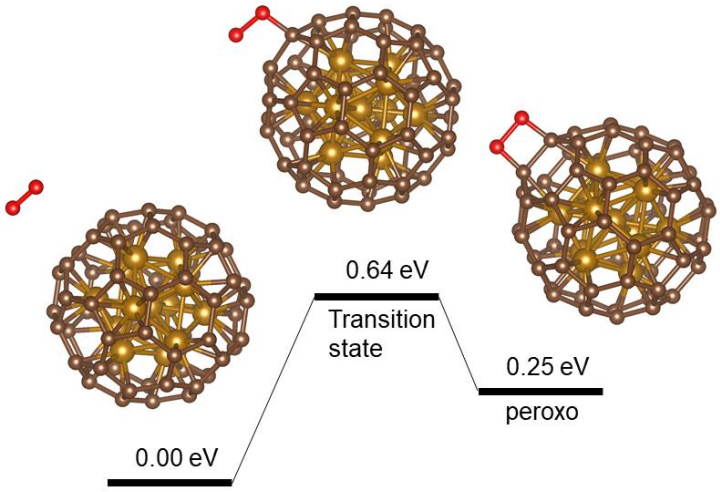


**Figure 1.** Molecular oxygen interaction with C60@Fe13 obtained with the NEB method.