The growth of economies has spurred an increase in energy demands and thus great interests in enhancing the electrochemical performance of various renewable energy applications such as fuel cells. Intensive research efforts have been undertaken in developing new catalysts to enhance the kinetics of oxidation and reduction reactions of compounds of interest. For this purpose metal-doped graphene hybrid materials have been explored, but with too much focus on noble metals, which are limited by their low availability and high costs, so transition metals may serve as promising alternatives [1,2].

In this work we present a study based on the Density Functional Theory as Gaussian09 program code, a sheet of graphene doped with 3d, 4d and 5d group transition metals. The hybrid PBE1PBE functional method was used and the effective-core-potential LANL2DZ for metal atoms and the 6-31G ++ (d) basis for the carbon and hydrogen atoms.

Our results indicate that the oxygen dissociation barrier decreases in doped systems regarding pure graphene sheet. This improved catalytic activity is allocated to the electronic and structural properties that promote doped with transition metals to a graphene sheet. From this result it can be considered doped graphene as a promising catalyst to the oxygen reduction reaction.

**Keywords:** Catalyst, Hybrid nanomaterial, Oxygen

**References:**


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