

Abstract Submitted
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Catalytic activity of transition metal-N₄ moieties in graphene toward the oxygen reduction reaction: A DFT study¹ WALTER ORELLANA, Universidad Andres Bello — The search for non-precious metal cathode catalysts for the oxygen reduction reaction (ORR) that replace platinum in proton exchange membrane fuel cells is one of the main challenges toward the use of hydrogen as clean energy for transportation. Most current works on ORR catalysts focuses on N-coordinated iron in a carbon matrix. Although the nature of the active site is still a mystery, different carbon-supported Fe-N_x active sites have been proposed. In this work, The O₂ dissociation after the interaction with the metal center of M-N₄ moieties in graphene (with M = Mn, Fe, and Co) are addressed by density functional theory calculations. Both, saddle points and minimum energy paths for the ORR in the allowed spin channels have been identified. Our results show that the Mn-N₄ center in graphene exhibits the lowest activation barrier in all spin channel, less than 1 eV, suggesting improved ORR activity, while for Fe-N₄ and Co-N₄ they range between 1.2 and 1.6 eV. Our calculations suggest that the O₂ dissociation would proceed through different spin channel which would increase the reaction rate, particularly for Mn-O₂ and Fe-O₂ moieties. We also investigate energetically favorable routes to incorporate the M-N₄ centers in graphene.

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