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Theoretical Study of Ru-Organometallic Compounds-Functionalized Grapheneas Catalyst Supports for Low-Temperature Fuel Cells.

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ABSTRACT

Nanostructured compounds such as carbon nanotubes (CNT), graphene (Gr) and ordered mesoporous carbon (OMC) have proven to be excellent supports to homogenously disperse electrocatalyst for fuel cell applications. However, the surface of these carbon materials has to be functionalized in order to properly anchor nanoparticles. Typically, aqua regia has been used to chemically modify the surface of the supports. In this work, the functionalization of graphene with ruthenium organometallic compounds (OM-Ru) has been studied using density functional theory (DFT) calculations. The OM-Ru complexes have ligands such as η^6-arene, -OH, -NR_2, -COOH and other polar groups that can promote the formation of surface functional groups on the graphene support to anchor Pt nanoparticles. Furthermore, it has been hypothesized that metallic Ru nanoparticles can be formed after functionalization and interact with Pt to create bimetallic phases. Thus, a synergetic effect at the graphene surface can be expected. The Pt/Gr electrocatalysts will be tested as anode materials for the Methanol and Ethanol Oxidation Reaction.

Keywords: Graphene supports; ruthenium organometallic compounds; functionalization; DFT; fuel cells.