Abstract Submitted
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Fe-Porphyrin adsorbed on single-wall carbon nanotubes for heterogeneous catalysis[1] WALTER ORELLANA, IGOR RUIZ-TAGLE, Universidad Andres Bello — We study the stability and electronic properties of Fe-Porphyrin (FeP) attached on pristine and defective (with a vacancy) single-wall carbon nanotubes (CNTs) by density functional theory calculations and molecular dynamic simulations. We investigate the CNT-FeP systems as a catalyst for the oxygen reduction reaction. Different configurations for the attached FeP were analyzed considering both physisorption and chemisorption. Metallic and semiconducting CNTs of about 1.1-nm in diameter are our model systems. Our results show that on pristine CNTs, FeP is physisorbed with binding energies of about 1.7 eV. Whereas, chemisorbed FeP (sp^3 and sp^2 hybridizations) have binding energies within 2.3-4.7 eV. Our molecular dynamic simulations show that these binding energies increase slightly at room temperature. The electronic band structures of the CNT-FeP systems preserve the CNT electronic characters, however, in (14,0)-FeP the band gap is reduced up to 0.03 eV, suggesting that this system behaves as an electron acceptor. The interaction between the O_2 molecule and the Fe atom of the FeP-CNT systems is also discussed.

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