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Fe-Porphyrin adsorbed and single-wall carbon nanotubes for heterogeneous catalysis

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Abstract – In this work we investigate the electronic properties of Fe-Porphyrin (FeP) attached onto single-wall carbon nanotubes (CNTs), exploring their use in heterogeneous catalysis. Different configurations for FePs were analyzed considering both physisorption and chemisorption.

We explore the stability and electronic properties of Fe-Porphyrin (FeP) attached on pristine and defective (with a single vacancy) single-wall carbon nanotubes (CNTs). Different configurations for FeP were analyzed considering both physisorption and chemisorption, exploring their possible use in heterogeneous catalysis for the O2 reduction [1,2]. Our theoretical approach is based on the density functional theory within the local spin-density approximation. We consider zigzag (14,0) and armchair (8,8) CNTs of about 11 Å in diameter, which have semiconducting and metallic characters respectively. Infinite CNTs are modeled with periodic boundary conditions along the nanotube axis. Our results show that on pristine CNTs, the FeP is adsorbed parallel to CNT surface (fig. 1a) with a mixture of both covalent (C-Fe) and Van der Waals (π-π stacking) interactions [3] with a binding energy of about 2 eV. We also attach a modified FeP (without an H atom) on both pristine (fig. 1b) and defective CNTs (fig. 1c). Here we observe a covalent C-C bond between the modified FeP and the nanotube, forming sp2 (with defective CNT) and sp3 (with pristine CNT) hybridization, where binding energies are found to be of 5 and 3 eV, respectively. The spin-resolved band structure of the physisorbed (14,0)-FeP system shows hybridized orbitals in the bandgap, which is reduced to 0.03 eV, suggesting that the system could behave as an electron donor. Whereas that, the chemisorbed (8,8)-FeP systems have a metallic behavior. These results suggest that FeP-CNT nanoassemblies could be used in catalytic processes.

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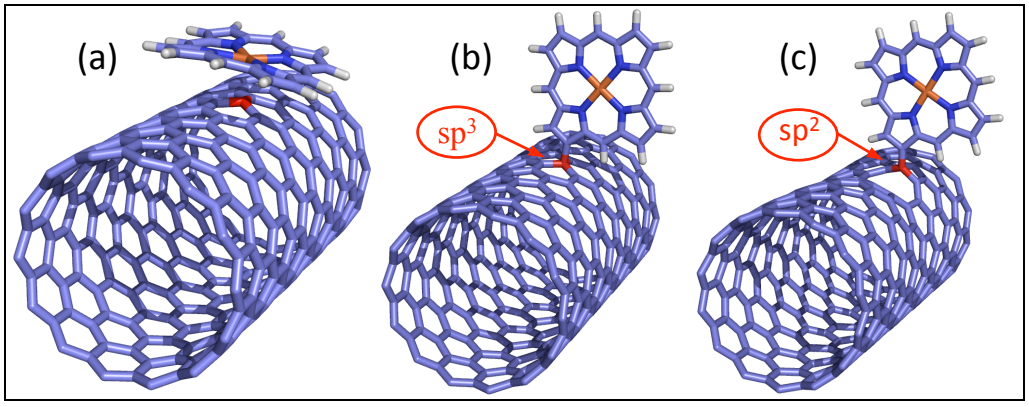

Figure 1 Geometries under study: (a) CNT (14,0) parallel adsorbed FeP, (b) CNT (14,0) normal attached modified FeP and (c) Defective CNT (14,0) normal attached modified FeP.

References

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