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Structural and electronic properties of $FeCl_3$ and CrO_3 interacting with GaP nanotubes from DFT calculations

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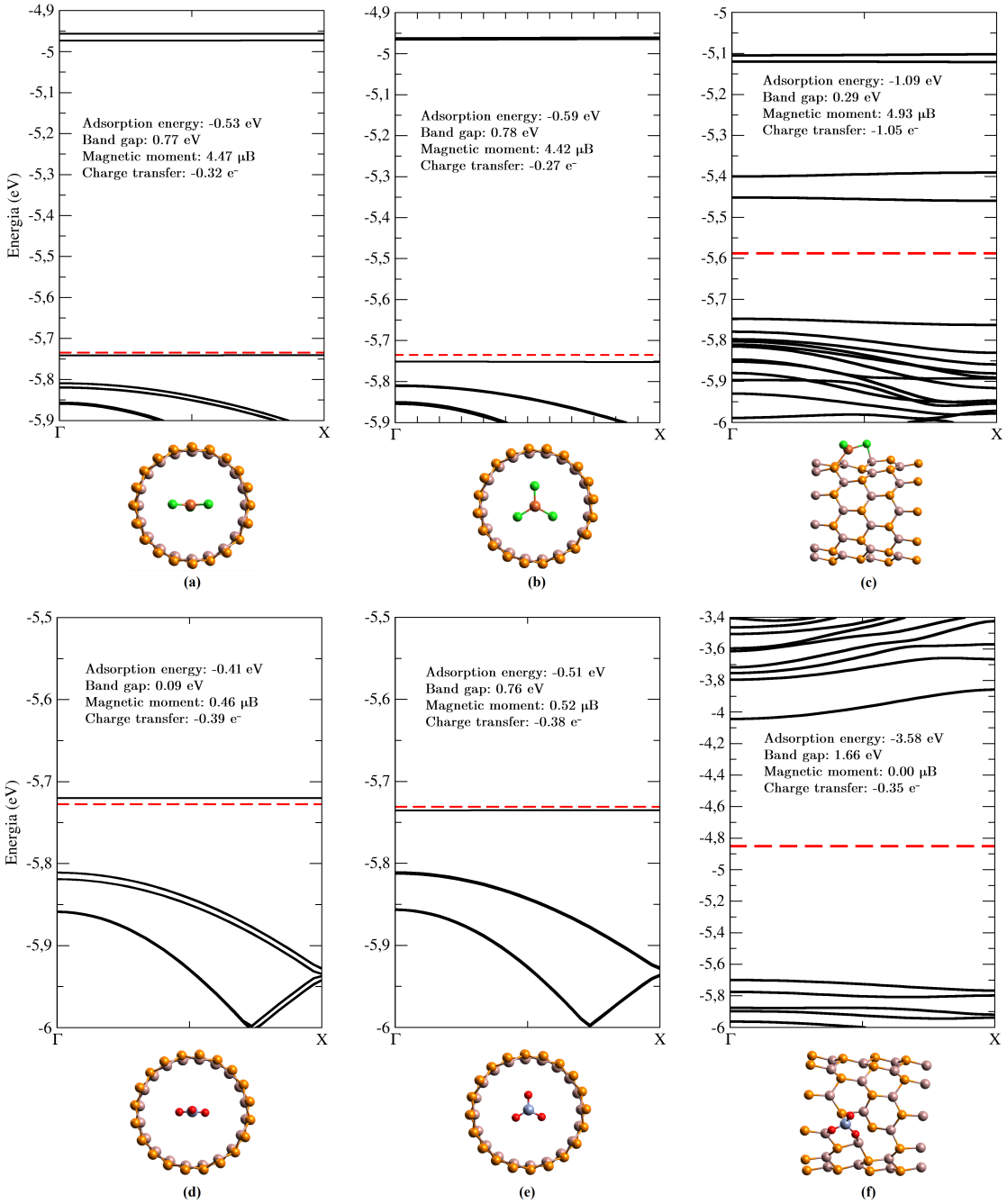

Figure 1: Electronic and energetic properties of the intermediate stability structures found in some systems with the GaP nanotube interacting with $FeCl_3$ and CrO_3, in which (a) were obtained in the initial configuration I for $FeCl_3$, (b) in the initial configuration II for $FeCl_3$, (c) in the initial configuration VIII for $FeCl_3$, (d) in the initial configuration I for CrO_3, (e) in the initial configuration II for CrO_3 and (f) in the initial configuration VIII for CrO_3. The illustration of each structure is represented at the bottom, where the light orange, light pink, dark orange, green, gray and red balls represent the atoms Ga, P, Fe, Cl, Cr and O, respectively. And at the top, the band structure of each system is plotted containing the adsorption energy, band gap, magnetic moment and charge transfer (from nanotube to the compound) of each structure. The Fermi level is represented by the horizontal dotted red line. The adsorption energies shown are with the BSSE correction.

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