Early stages of Ti-O clusters' growth on SWNTs by ab initio calculations

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We performed Density Functional Theory calculations to study the early stages of growth of Ti-O tetrahedral (Th) and octahedral (Oh) clusters, dimmers or trimmers on Single Wall Carbon Nanotubes (SWNT (8,0) and (5,5)). We found that Th may exist in several conformations with well localized electronic states, mainly below -1.5eV, whereas Oh are less stable and may be transformed to Th. In line with experimental suggestions, the Th could be considered as active, due to the localization of charge distribution and the emergence of C dangling bonds at the Fermi level. On the contrary, the Oh retains the pure SWNT C_{2p}-C_{2p} π-like features. Nevertheless, all Ti-O clusters, exhibit new Ti_{3d} states above -3eV revealing the expected O_{2p} - C_{2p} and interestingly Ti_{3d} - C_{2p} hybridizations, thus altering the (8,0) semiconducting character. From all edge-sharing clusters, we found that the linear Rutile-like octahedral trimmer (OhOhOh) favors the parallel to the zigzag alignment, while equiprobable growth for the two Ti-O phases, with small tendency towards spinal anatase-like OhOhOh, is expected for clusters vertically to SWNT. These results are in line with the Ti-O deposition on a multi wall carbon nanotube. These results could enlighten the early stages of growth of Ti-O on SWNT providing useful information in the field of nanoelectronics and nanotechnology.

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