Defects distribution and geometrical disturbances in Carbon Nanotube Heterojuntions

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The relative stability of a family of carbon nanotubes (CNT) with defects has been investigated theoretically with first-principles density functional theory (DFT) calculations, B3LYP/6-31G*. A set of (12,0)-(8,0) CNT heterojunctions with an increasing number (n=1-4) of pentagon/heptagon defects were studied systematically in different arrangements, and the results compared with a set of small graphene defective fragments. The strucutures were contructed with CoNTub Software.[1][2] In addition, tubular structures with two pairs of defects distributed variedly (along and around the CNT) with increasing distances were considered. Within the defective structures, that containing the well-known Stone-Wales defect resulted the most stable one. However, if more than two pairs of defects coexist, situations where the defects appear together seem to be preferred, in sharp contrast to the isolated pentagon rule (IPR) for fullerenes, although this is in accordance with some previous works on this topic. The junctions studied here constitute different arrangements that allow us to discuss which effects (geometric and energetic) arise from the particular positions and orientations of the defects in nanotubes. Moreover, a hefty correlation between the energetic stability and the geometric deformation was found, measured with the average pyramidalization angle (POAV) and the average trigonal deformation (D_{120}), as well as Main Bond Length (MBL) and Ring Bond Dispersion (RBD), which has been already demonstrated useful parameters in analyzing geometrical features in graphite-like structures[3]. For such purpose, the different contributions to molecular strain were analyzed with the TubeAnalyzer software.

References

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Figures