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Selective Edge Filling of Collapsed Carbon Nanotubes for Nanoelectronics: An ab-initio study

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The spontaneous collapse of large-diameter single carbon nanotubes (SWCNTs) generates a new class of low dimensional structures, known as collapsed 'dogbone' nanotubes. Several experimental works showed that the final configuration of collapsed tubes is composed by two flat nanoribbons, whose edges are closed forming chemical bonds like the standard carbon nanotubes. Our first-principle investigation based on the Density Functional Theory (DFT) revealed how these flattened tubes become more stable than its own cylindrical counterpart when a given diameter threshold is exceeded. A peculiarity of these hybrid systems between bilayer graphene and SWNTs due to their unique architecture is the possibility to fill the edge cavities with different molecules. The radial deformation of filled nanotubes is driven by changes in the charge transfer process between molecular species and surrounding carbon edge channels. The edge filling implies Coulomb interactions between molecules and molecules and CNT-like zone at the edges. The filled cavities induce doping effect on the collapsed nanotubes without the introduction of defects and/or scattering centres with really significant improvement of the electrical conductivity. Such innovative systems represent a rising star on the horizon of nanomaterials science, because of peculiar mechanical and electronic properties, opening the path to promising deformed graphene based on high-performance nanoscale devices.

Choix de session parallèle

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