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Selective Edge Filling of Collapsed Carbon Nanotubes for Field Effect Transistors

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Recently innovative methods have been proposed for the creation of a novel generation of high-quality bilayer graphene nanoribbons (B-GNRs) presented as superior candidates for the building of a better class of electronic devices [1]. These nanoribbons can be obtained from self-collapsing of single-walled carbon nanotubes (SWCNTs), whose structure is composed of two strained bulbs connected by a central region similar to bilayer graphene. The thermodynamics stability for collapse strongly depend on the computational method and the initial configuration between the two layers of graphene (see Figure 1(a)) [2]. The structural phase transition from cylindrical geometry to collapsed structure induces a second electronic phase transition as a result of the opening of a small energy gap, which varies with the size of the nanotube, the lattice registry and the chirality tube (see Figure 1(b)) [3]. The fundamental feature of such hybrid systems between SWCNT and B-GNR would be the possibility of filling cavities with different molecules for the modulation of conductivity with charge doping (see Figure 1(c)). According to the *first-principle* analysis based on the Density Functional Theory we can study and understand the electronic properties of these deformed tubes, which can be used for the future electronics.

References

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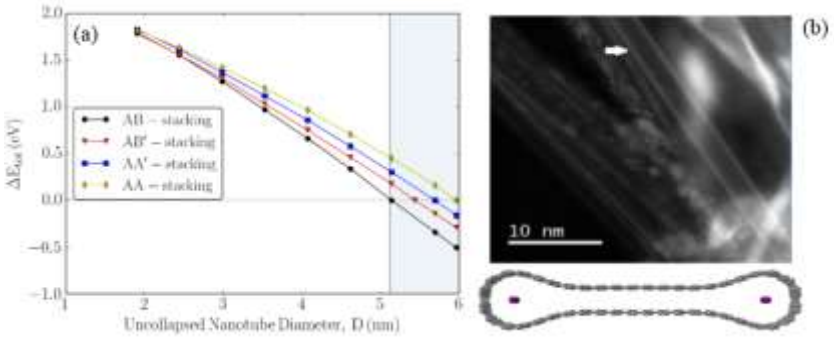

Figure 1: *(a) DFT-vdW calculated threshold diameter for pure armchair (n,n) single-walled carbon nanotubes to collapse. Datasets represent interlayer shearing of the same collapsed tube, resulting in different interlayer stacking in both central bilayer graphene region and curved edge bulbs, AB (black), AB' (red), AA' (blue), and AA (yellow). (b) Scanning Transmission Electronic Microscopy image of Iodine@filled Collapsed CNTs and its simulated geometry.*