Pyridine- and $C_{10}H_{10}BN$-based nanotubes: A route to always semiconducting NTs

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The synthesis of carbon nanotubes (CNTs) doped with different impurities is a way to tailor their electronic properties. Several groups have achieved high nitrogen concentration with CVD techniques [1, 2]. Recently Chen *et al.* [3] have demonstrated the Vapor-Liquid-Solid (VLS) fabrication of nanotubes with an ultra-high N concentration and control over the N arrangements, based on a pyridine [see Fig. 1.a)] precursor gas and an Fe–Co catalyst.

We have performed first-principles calculations with the SIESTA [4] program showing that the metallic or semiconducting character of pyridine-based nanotubes will depend on the specific arrangement of the N atoms within and the chirality of the NT.

On the other hand, changing to a different precursor where the extra nitrogen atoms are compensated by boron atoms, such as a borabenzene-pyridine adduct [5, 6] [Fig. 1.b)], we show that a gap will open for pristine metallic CNTs (Fig. 2), while for pristine semiconducting CNTs the gap will be reduced by some amount (Fig. 3), but maintaining the semiconducting character.

Therefore, a $C_{10}BN$ nanotube (CBNNT) would always be semiconductor, easing the fabrication of CNT-based circuitry.

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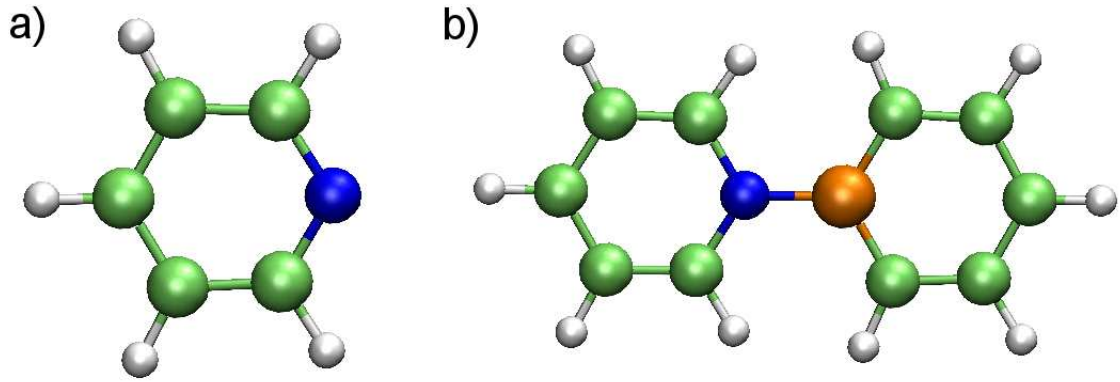

FIG. 1: a) Pyridine (C_5H_5N) molecule. b) Pyridine-borabenzene adduct ($C_{10}H_{10}BN$) molecule. The blue (dark) atom corresponds to nitrogen.

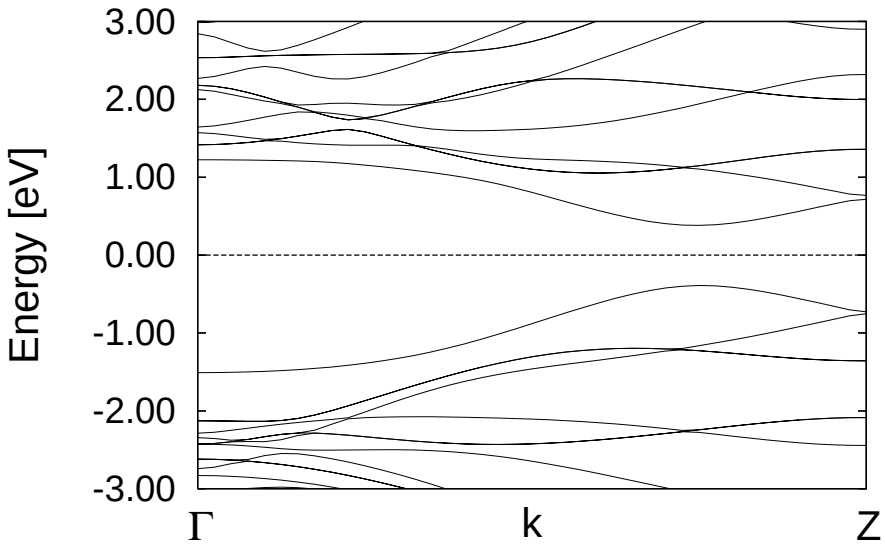

FIG. 2: Band structure of a (6,6) CBNNT showing the opening of a gap, where the CNT analog would be metallic. The dashed line corresponds to the Fermi level.

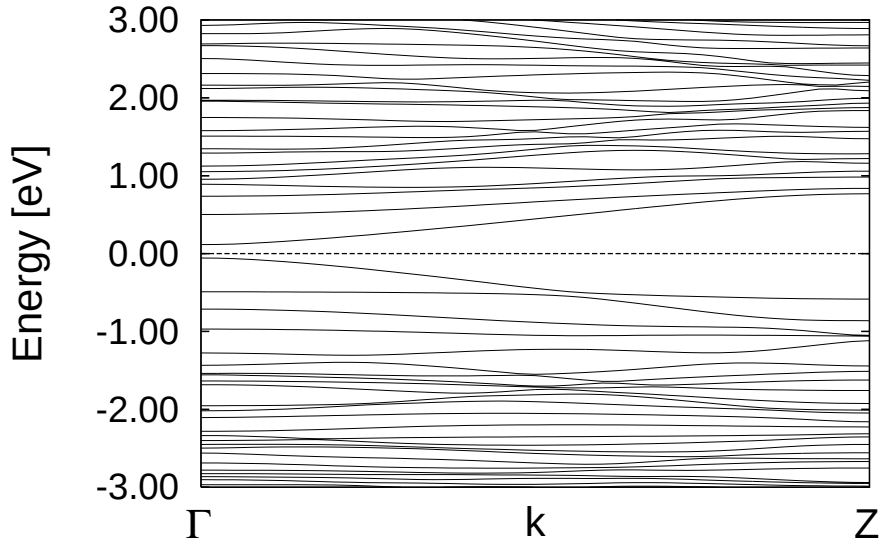

FIG. 3: Band structure of a (10,0) CBNNT showing the existence of a gap, which is reduced in numerical value with respect to its pristine CNT analogue.