Local semiconducting transition in armchair carbon nanotubes

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Assuming the possibility of chirality-sensitive selection of single wall carbon nanotubes (SWCNT) the next step towards single-SWCNT nanoelectronic devices is the creation of rectifying metal-semiconductor junctions. Occasionally, this kind of junctions are realized due to pentagon-heptagon defects making a seamless junction between nanotubes of different chiralities [1] Another route could be to modify the electronic bandstructure of a single SWCNT spatially by functionalization with defects, adatoms, or molecules. [2,3] We have studied recently how periodic bi-site perturbations on the metallic armchair SWCN turn them locally semiconducting. [4]

We have performed bandstructure and electronic transport calculations within the density functional theory (DFT) implemented in SIESTA [5] and Transiesta [6] programs and within the basic tight-binding method for an armchair SWCNT with periodically adsorbed hydrogen clusters (Figure 1). Figure 2 shows that for infinitely repeated clusters a bandgap opens when the distances $\vec{R}$ between adjacent bi-site perturbations fulfill the condition

$$\vec{R} = p\vec{a} + q\vec{b}, \qquad p - q = 3M, \qquad M \in Z,$$

where $\vec{a}$ and $\vec{b}$ are unit vectors given in Figure 1. Figure 3 shows how the electron transmission coefficient for $M = 6$ ($M = 5$) decays (saturates to the ideal value) at the Fermi level as the length (N) of the periodically decorated section of the armchair SWCNT increases. The opening of the band gap and the decay of the transmission can be understood as the result of the folding of the band intersection point to the Γ point with periodic perturbations or as the constructive interference of backscattered electrons when the distance between the perturbations along the tube axis is a multiple of half of the Fermi wavelength.

We have studied also the robustness of the band gap opening against variations in the types and positions of perturbing cluster species. The gap opening phenomenon is proposed as a means for creating single-SWCNT electronic devices.

References

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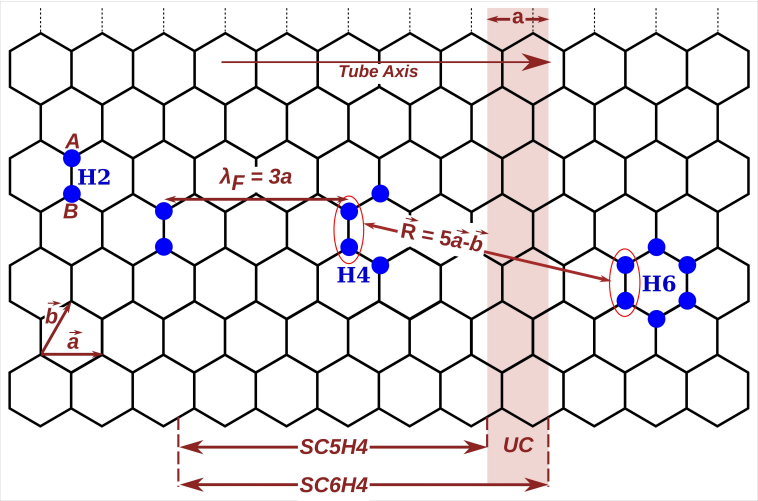

Figure 1. Hydrogen clusters H2, H4, and H6 on an (8,8) armchair SWCNT. The unit cell UC of the pristine tube and the supercells SC5H4 and SC6H4 are defined.

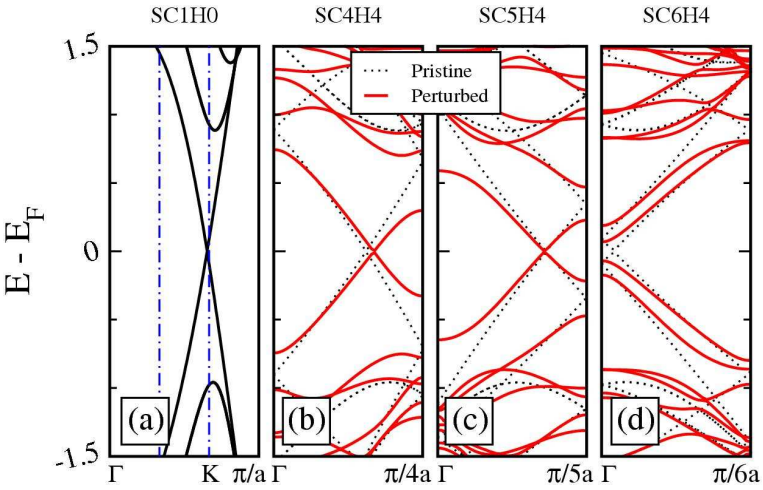

Figure 2. Bandstructures of a pristine armchair SWCNT (SC1H0) and tubes with periodically adsorbed hydrogen clusters (SC4H4, SC5H4, SC6H4).

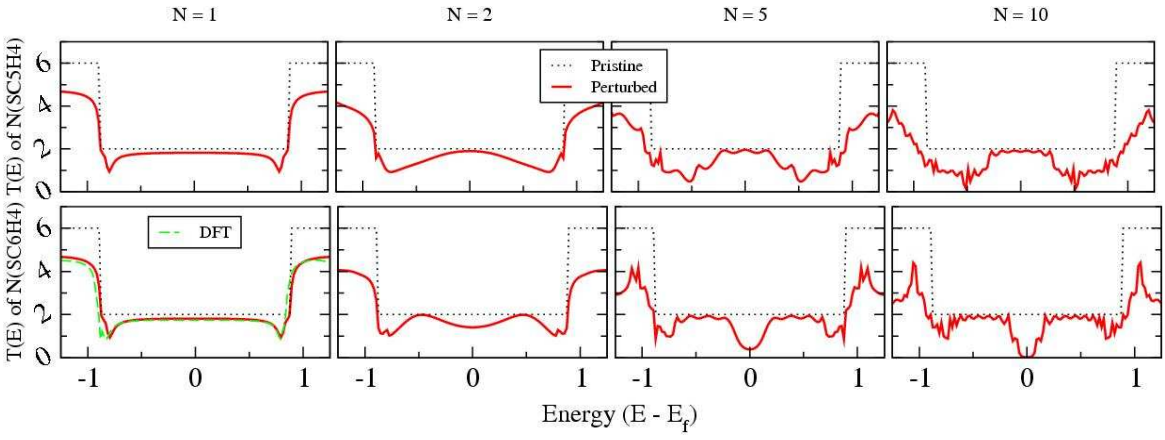

Figure 3.Transmission coefficient of an armchair SWCNT containing a section periodically decorated with H4 clusters. The upper and lower panels correspond to the SC5H4 and SC6H4 supercells, respectively. The length of the decorated section increases from one (N=1) to ten (N=10) supercells.