–Supporting Information–

From Cyclic Nanobelts to Single-Walled Carbon Nanotubes: Disclosing the Evolution of their Electronic Structure with the Help of Theoretical Methods

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1 Physics provided by the tight-binding method

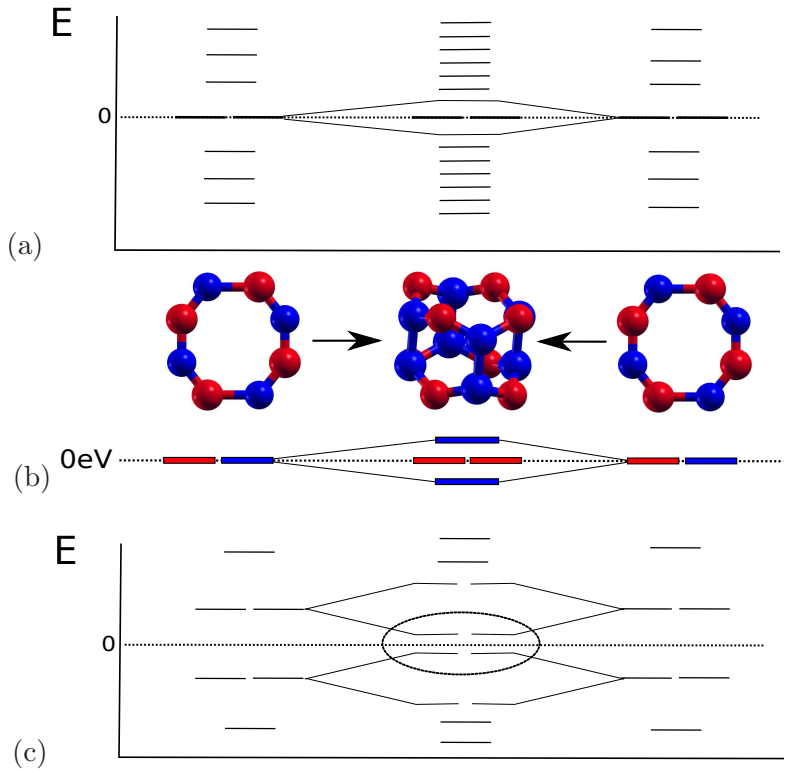

Figure S1: Sketch showing the formation of zero-energy modes when even (a-b) and odd (c) symmetrical and equivalent parts of $[n]$CC are bound together.

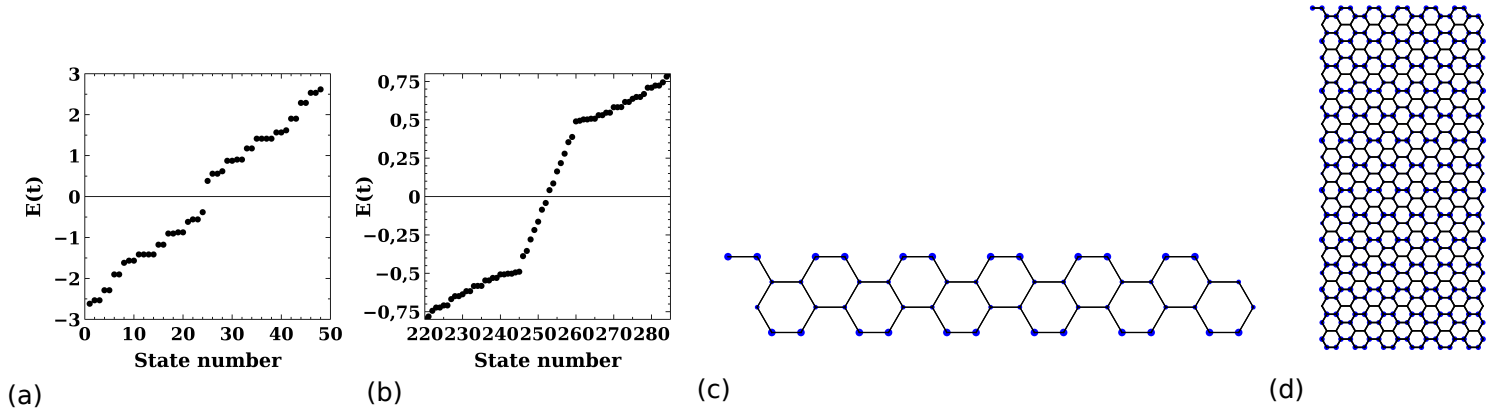

Figure S2: Tight-binding eigenvalue spectra for [12]CPH with (a) $L = 1$, (b) $L = 20$, as well as the plot of their corresponding HOMO –(c) and (d)–.

2 Energy magnitudes by the RAS-SF method

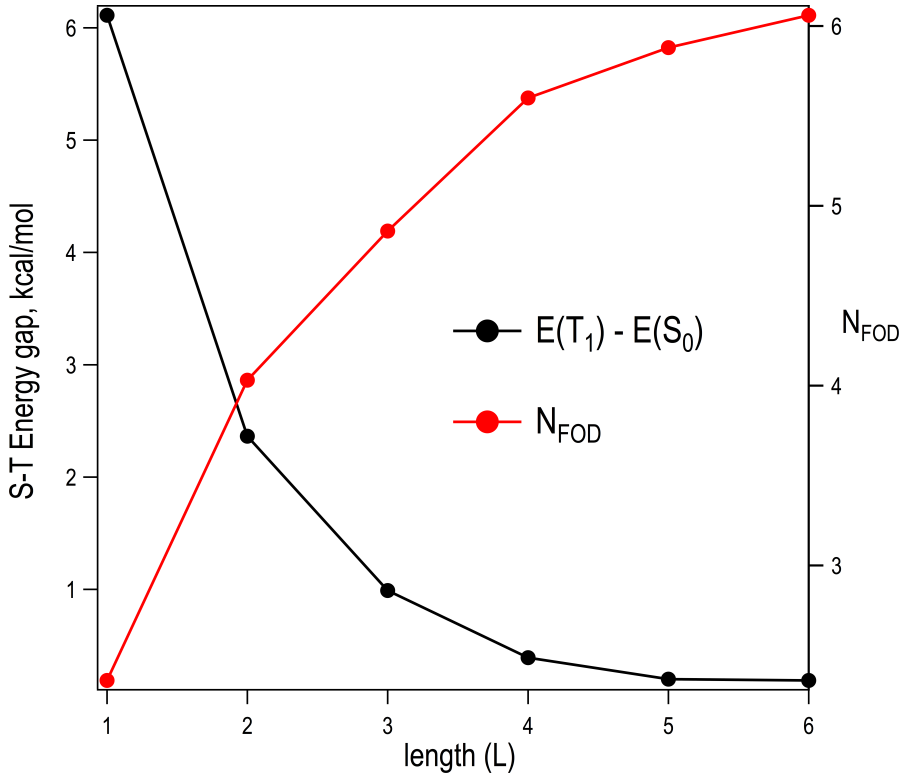

Figure S3: Evolution of the ΔE_{ST} and N_{FOD} values obtained at the RAS-SF/6-31G(d) level as a function of the nanotube size ($L = 1-6$) for [12]CC.

3 Topology of the FT-DFT calculated FOD density for increasingly longer nanobelts

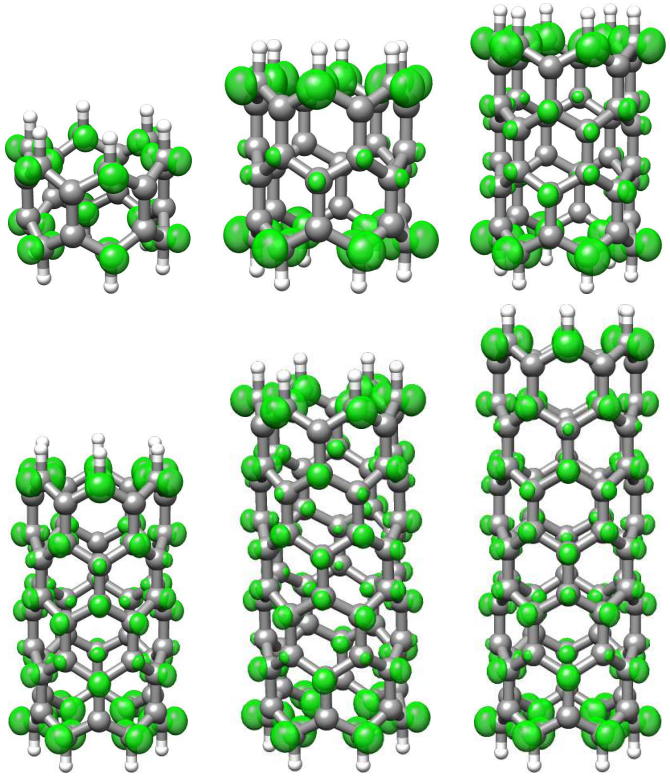

Figure S4: Chemical structures and plots ($\sigma = 0.005$ e/bohr^3) of the FOD density as obtained from the FT-DFT method, for the set of [6]CC compounds ($L = 1 - 6$, from left to right for increasing values of L).

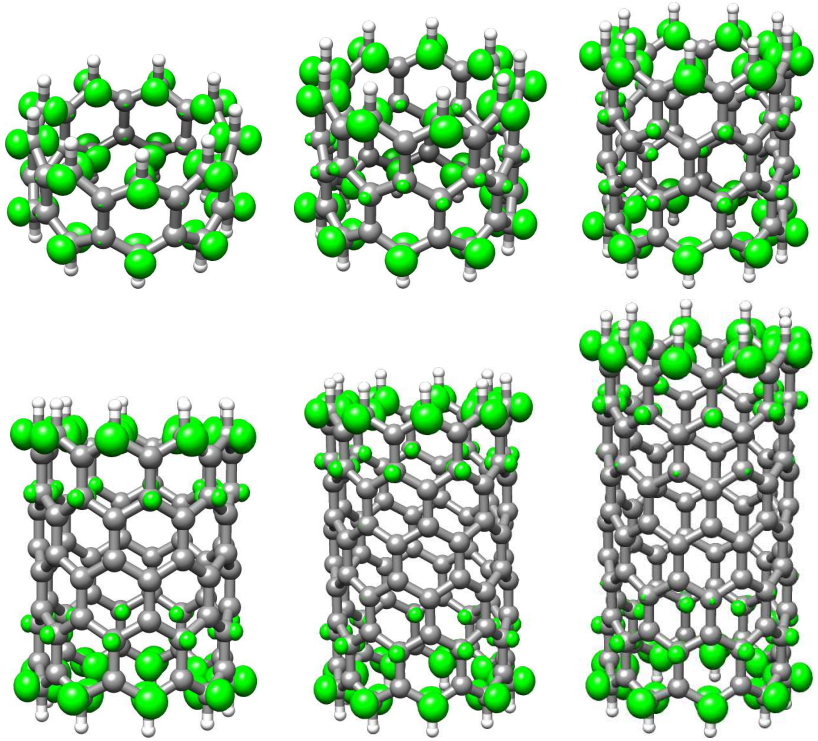

Figure S5: Chemical structures and plots ($\sigma = 0.005$ e/bohr^3) of the FOD density as obtained from the FT-DFT method, for the set of [9]CC compounds ($L = 1 - 6$, from left to right for increasing values of L).

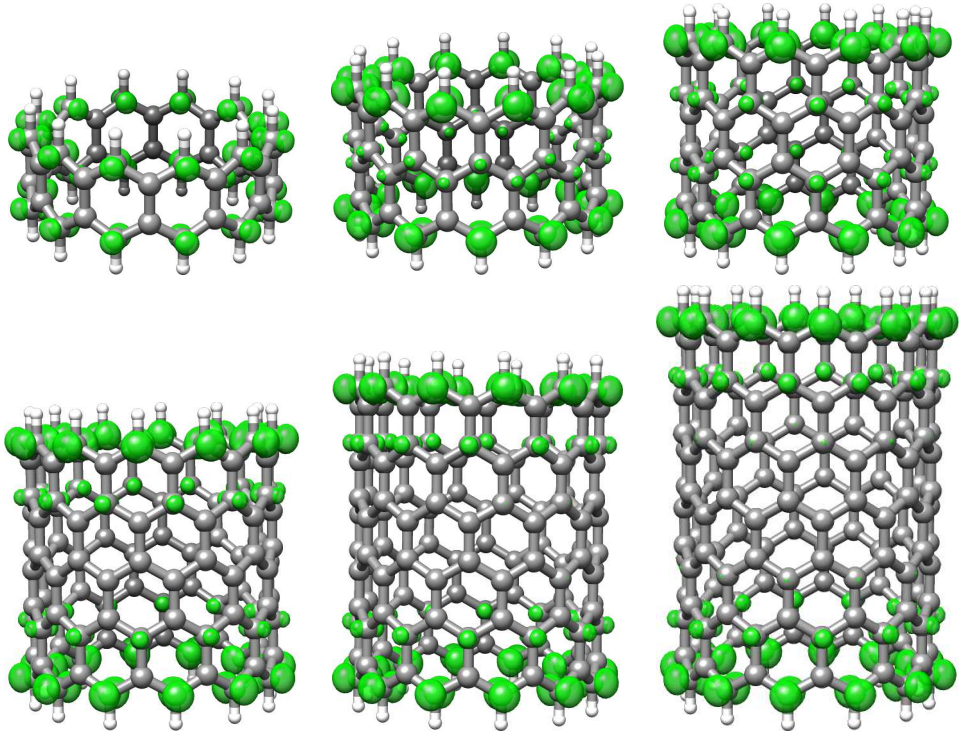

Figure S6: Chemical structures and plots ($\sigma = 0.005$ e/bohr^3) of the FOD density as obtained from the FT-DFT method, for the set of [12]CC compounds ($L = 1 - 6$, from left to right for increasing values of L).

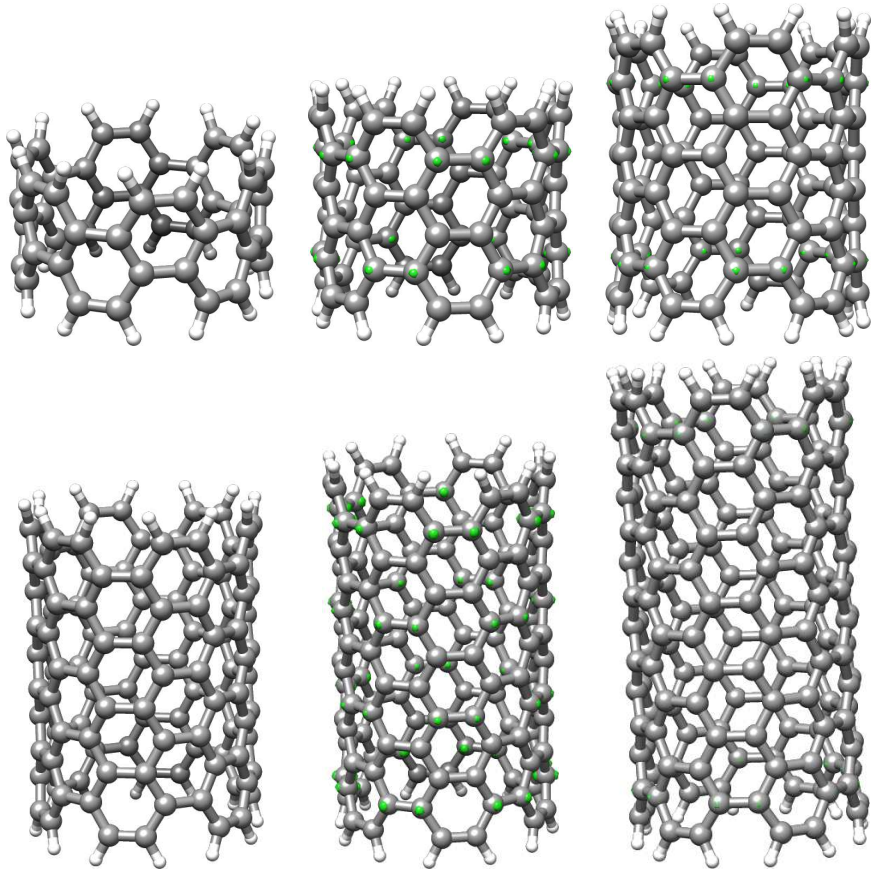

Figure S7: Chemical structures and plots ($\sigma = 0.005$ e/bohr^3) of the FOD density as obtained from the FT-DFT method, for the set of [12]CPH compounds ($L = 1 - 6$, from left to right for increasing values of L).

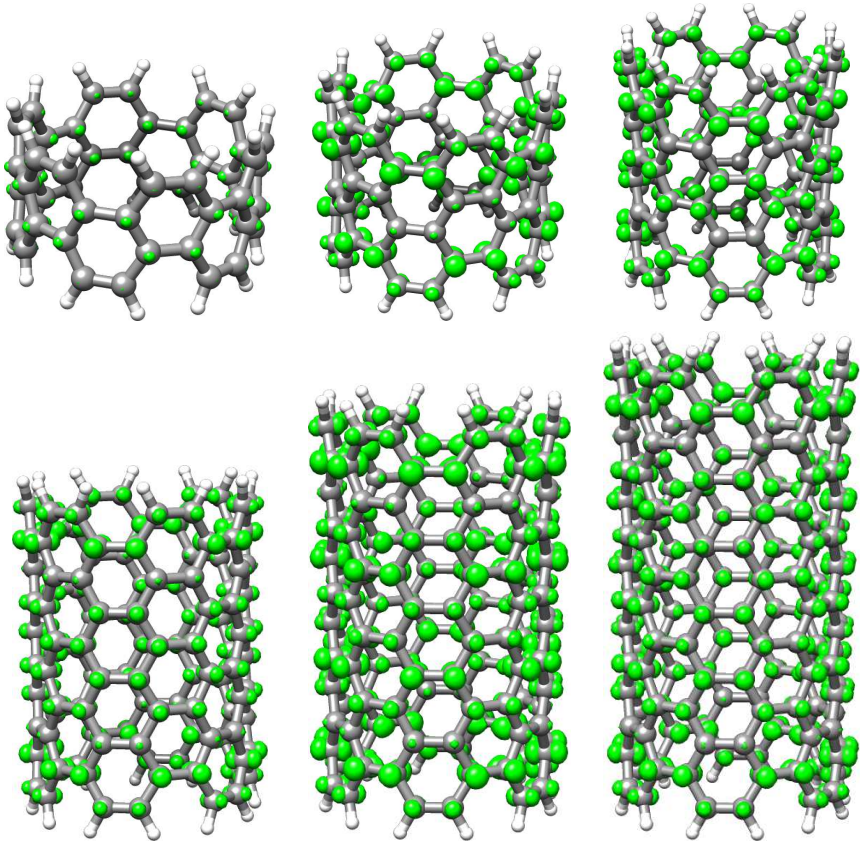

Figure S8: Chemical structures and plots ($\sigma = 0.002$ e/bohr^3) of the FOD density as obtained from the FT-DFT method, for the set of [12]CPH compounds ($L = 1 - 6$, from left to right for increasing values of L).

4 Topology of the RAS-SF calculated FOD density for increasingly longer nanobelts

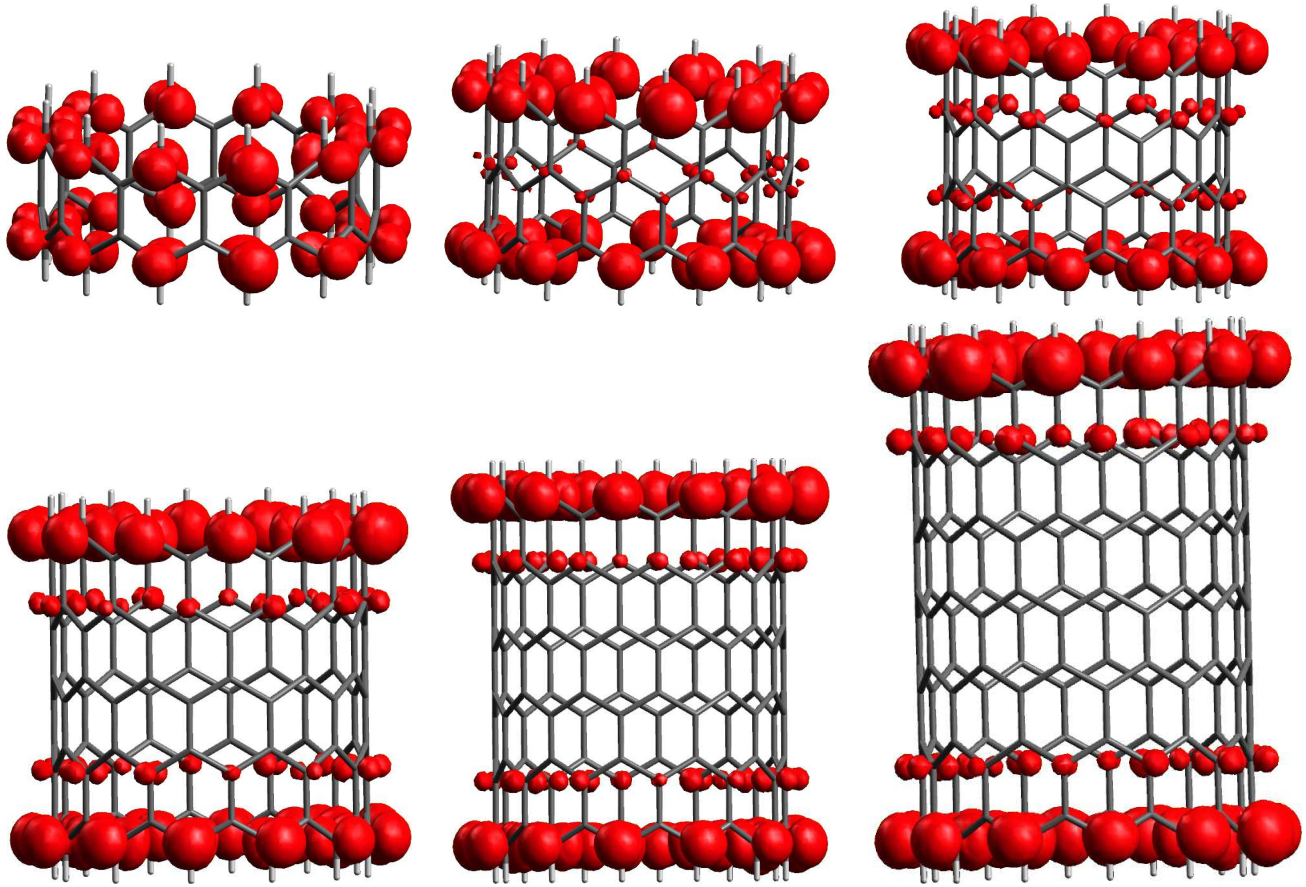

Figure S9: Chemical structures and plots ($\sigma = 0.002$ e/bohr^3) of FOD obtained with RAS-SF/6-31G(d), for the set of [12]CC compounds ($L = 1 - 6$, from left to right for increasing values of L).