Supporting Material

Strain-Controlled Magnetic Ordering in 2D Carbon Metamaterials

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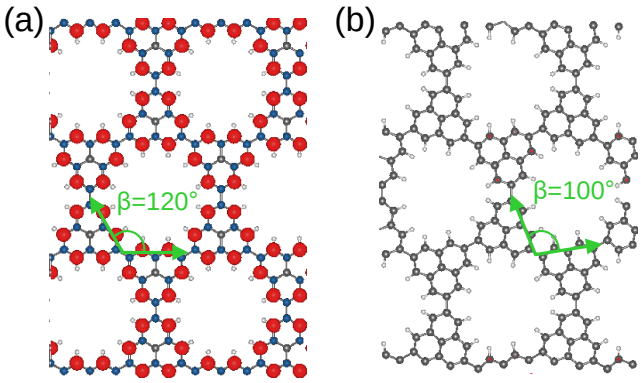

Figure S1: Spin polarized charge density $\rho_\uparrow - \rho_\downarrow$ in the $(C_{13}H_6\text{-}C_{13}H_6)_\infty$ polyphenalenyl lattice, with isosurfaces bounded by $+3\times10^{-3}$ e/Å^3 for the $\uparrow$ majority spin (red) and by -3×10^{-3} e/Å^3 for the $\downarrow$ minority spin (dark blue). The two values of the opening angle β shown are (a) $\beta = 120°$ and (b) $\beta = 100°$.

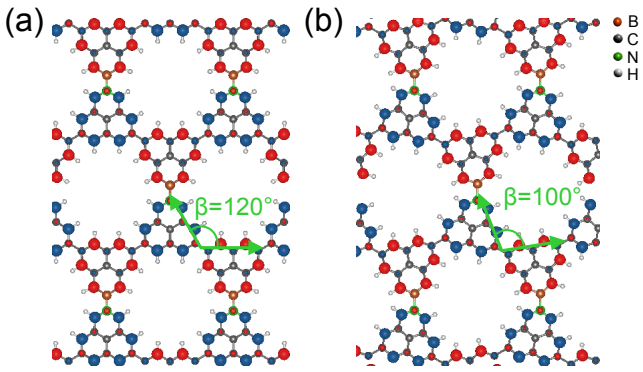

Figure S2: Spin polarized charge density $\rho_\uparrow - \rho_\downarrow$ in the B-N doped $(C_{12}H_6B\text{-}C_{12}H_6N)_\infty$ polyphenalenyl lattice, with isosurfaces bounded by $+2\times10^{-3}$ e/Å^3 for the $\uparrow$ spin (red) and by -2×10^{-3} e/Å^3 for the $\downarrow$ spin (dark blue). The two values of the opening angle β shown are (a) $\beta = 120°$ and (b) $\beta = 100°$.

Spin polarized charge density

The spin-polarized charge density $\rho_\uparrow - \rho_\downarrow$ of the $(C_{13}H_6\text{-}C_{13}H_6)_\infty$ polyphenalenyl lattice with two values of the orientational angle β is shown in Fig. S1. With the two spin polarizations being represented by different colors, we clearly see that the majority spin, represented by red, dominates the lattice, indicating that the $(C_{13}H_6\text{-}C_{13}H_6)_\infty$ system is ferromagnetic.

The spin-polarized charge density of the B–N doped $(C_{12}H_6B\text{-}C_{12}H_6N)_\infty$ polyphenalenyl lattice with two values of the orientational angle β is shown in Fig. S2. The two spin polarizations are distinguished by color. We clearly see the dominant color on the B-doped radical to be red, indicating that the majority state carries spin-up electrons. The dominant color on the N-doped radical is dark blue, indicating that the majority state carries spin-down electrons. With magnetic moments of opposite direction on adjacent phenalenyl radicals in the unit cell, the system is antiferromagnetic.

Comparing results for both systems for different values of the orientation angle β, we clearly see that the magnetization is very sensitive to β in the undoped system, as seen by comparing Figs. S1(a) and S1(b). The magnetic moment of the two sublattices in the doped system, represented in Fig. S2, is much less sensitive to β due to the charge depletion on the polar B–N bonds connecting the sublattices.