

Supplementary materials

Topological Phases, Local Magnetic Moments, and Spin Polarization Triggered by C_{558} -Line Defects in Armchair Graphene Nanoribbon

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I. THE 3P RULE OF BAND STRUCTURES

In this section, we introduce the periodic band structures related to the nanoribbon width, as shown in Fig. S1. Although we show the bands for only two periods, it is sufficient to observe the dispersion pattern of the bands within the $\Gamma - X$ interval. When $w = 3p + 2$, the pair of Dirac points appears in the k_x direction, while this property is not present for other widths of nanoribbons. It is worth noting that when the width w characterizing the nanoribbon is even, the symmetry of the system is different and the unit cell is rhombic, as shown in Fig. S1(h). However, this difference does not affect the properties of the system in the k_x direction. This periodicity is identical to that of the armchair nanoribbons. The reason for this is due to the interleaved C_{558} -line defects, which break the original periodicity and add a full wavelength, so that this armchair interface condition also exhibits three-periodicity in the defect structure, as is the case for other similar materials.

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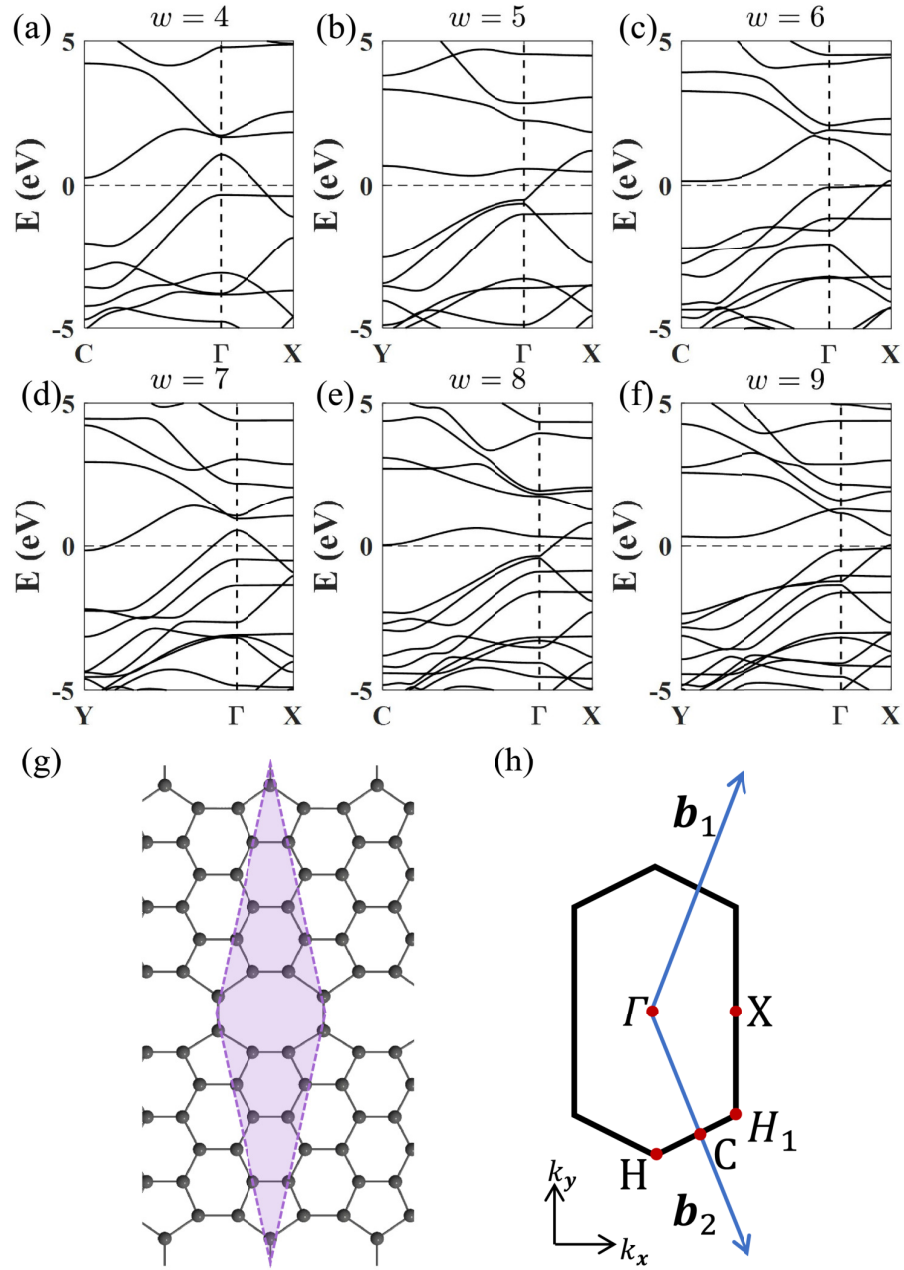


FIG. S1: (a-f) Band structures corresponding to $w = 4 \sim 9$. (g) If w is an even number, the form of a single cell; And the first Brillouin zone and its high symmetry point, b_1 and b_2 are two reciprocal basis vectors appearing in (h).