Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Family-dependent magnetism in atomic boron adsorbed armchair graphene nanoribbons

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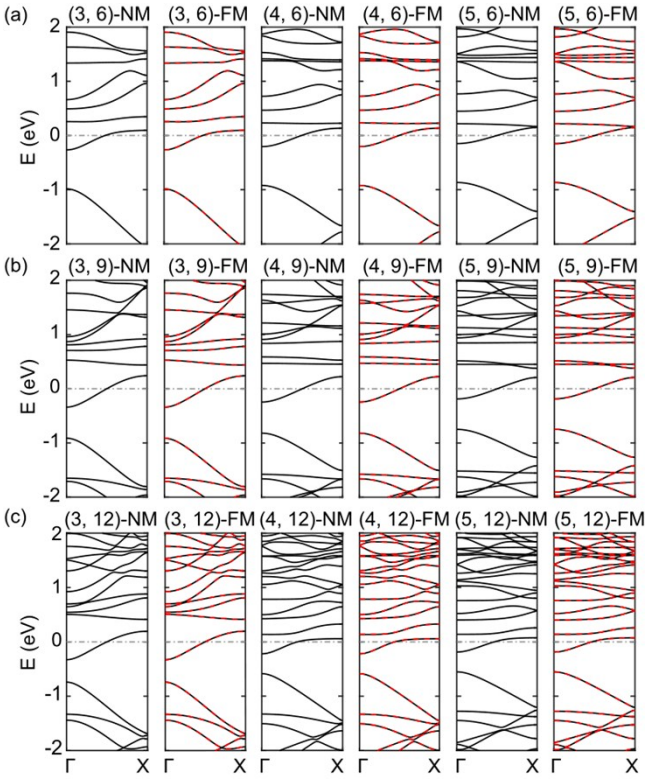

Figure S1 | Band structure of the B-AGNRs with width W = 6 (a), 9 (b), and 12 (c) in the family of W =3p, respectively, and the Fermi level is set zero.

Each ribbon possesses a partially-filled energy band (PFEB), which runs across the Fermi level of each ribbon with delocalization, and the B atom induced states locate above the Fermi level, resulting in nonmagnetic ground state.

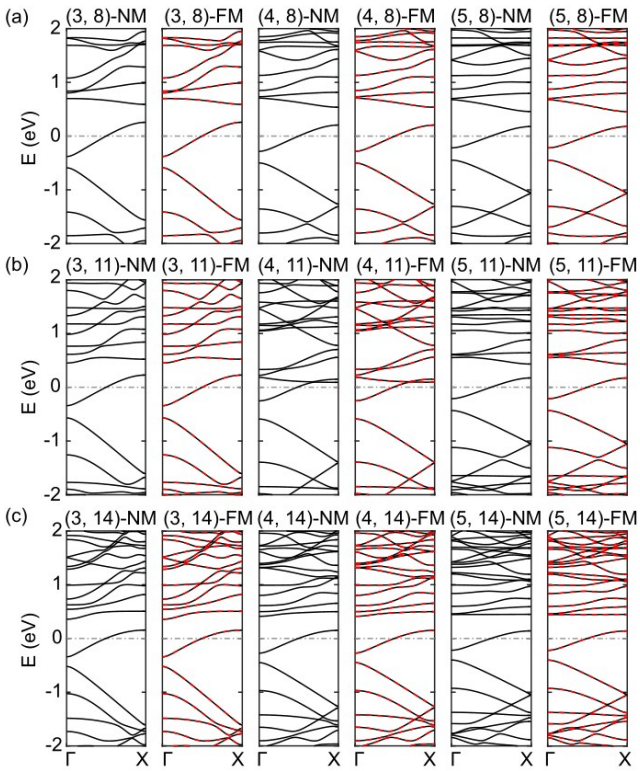

Figure S2 | Band structure of the B-AGNRs of width W = 8 (a), 11 (b), and 14 (c) in the family of W =3p+2, respectively, and the Fermi level is set zero.

Each ribbon possesses a partially-filled energy band (PFEB), which runs across the Fermi level of each ribbon with delocalization, and the B atom induced states locate above the Fermi level, resulting in nonmagnetic ground state.

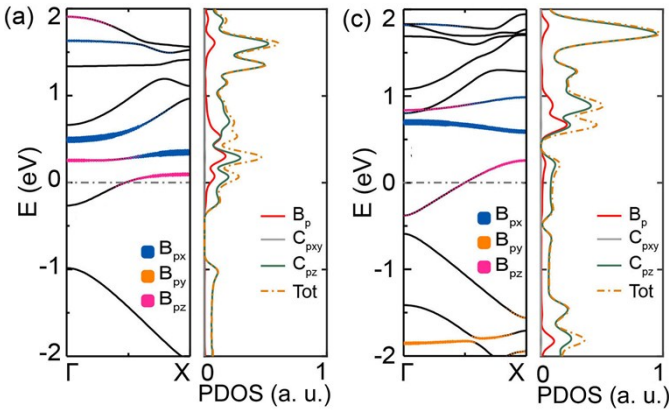

Figure S3 | Fat band structure and PDOS of the B-AGNRs with width W = 6 (a), and 8 (b) under nonmagnetic ground state.

Although the p_z orbital of B contributes the VBM, the VBM is delocalized. Although the system owns some localized states, they appear in CB region that is allowed and thus spin-splitting does not occur.

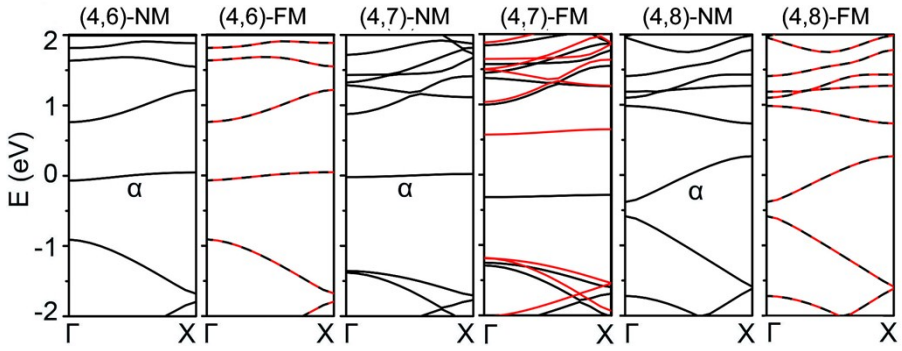

Figure S4 | The electronic band structures of the (4, 6), (4, 7), and (4, 8) B-AGNRs calculated by the Heyd-Scuseria-Ernzerhof (HSE06) screened hybrid functional.

One can see that spin-splitting occurs only in (4, 7) B-AGNR, which belongs to the family of W=3p+1, due to that it possesses a largely localized band right at the Fermi level under NM state. And a magnetic moment of 1.0 μ_B also presents at the FM ground state. Thus the same conclusion as predicted from GGA-PBE is reached in HSE06 framework.

Designing of graphene nanoribbon:

Both the theoretical and experimental studies proved that the properties of graphene nanoribbons (GNRs) are mainly dependent on their geometric structures [1,2]. Up to now, there exist two main types of methods for preparing GNRs with precise edge structures, namely top-down and bottom-up synthesis. For the top-down synthesis of GNRs, two typical methods have been proposed are realized in experiments. The one is to cut or etch graphene or graphite precursors into nanoribbons [3,4], and the other is to longitudinally unzip single-walled and multi-walled carbon nanotubes (CNTs) to produce GNRs[5,6]. For bottom-up preparing of GNRs, it starts with the rational design and self-assembly of small-molecule precursors [7-9]. This method can utilize a two-step polymerization sequence and then carry out cyclization dehydrogenation. The first case of bottom-up synthesis of atomically precise GNRs with width of W = 7 was published by researchers in 2010[7]. And ultranarrow AGNRs (W = 5) with precise edge structures have already been synthesized by Zhang et al in 2015[8].

References:

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