

## Supporting information for

# Electronic Structure and Magnetic Properties of Penta-Graphene Nanoribbons

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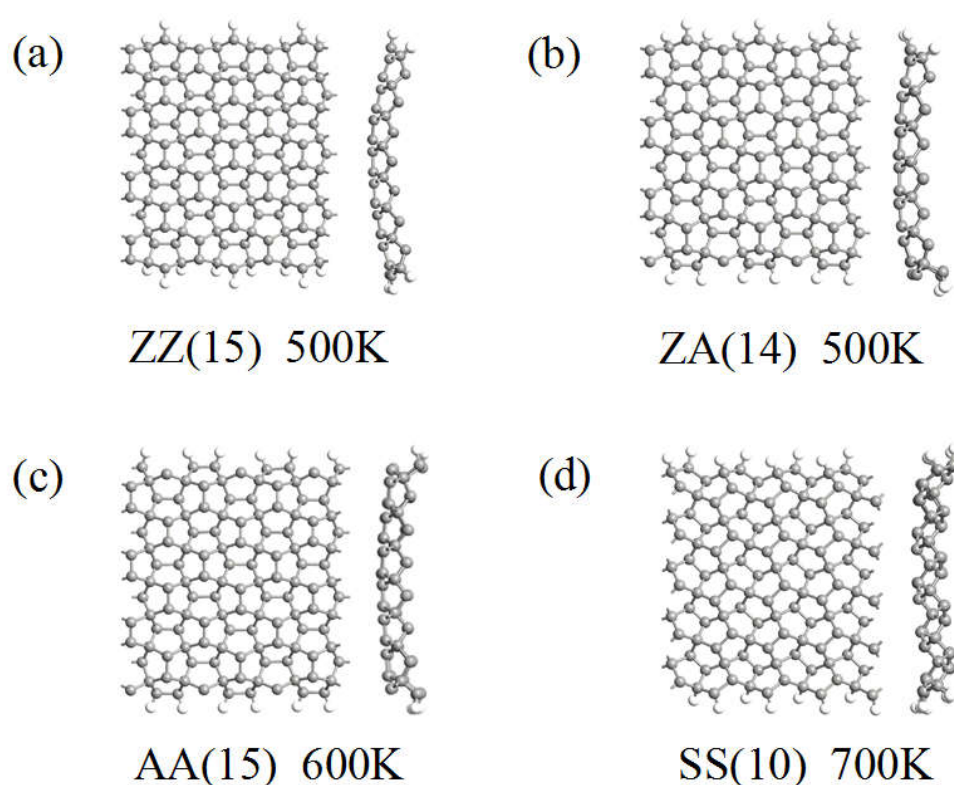


Fig.S1. BOMD simulations are performed to examine thermal stability of the P-GNRs..The small deformations occurring at 500K for ZZ (a )and ZA (b), at 600K for AA (c), and at 700K for SS (d) after 8 ps of simulation, but no edge reconstruction is observed.

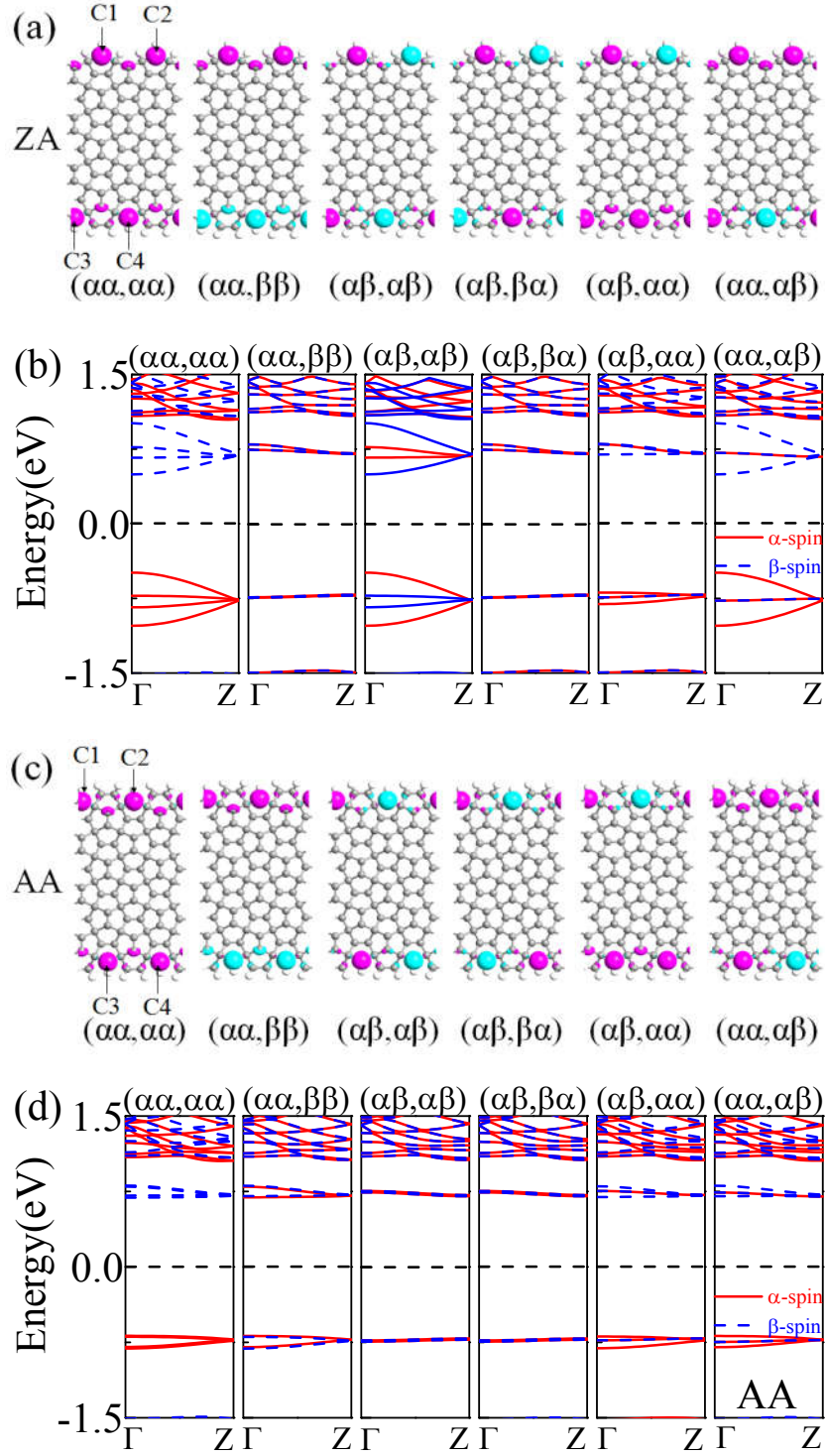


Fig.S2. Schematic of the six different magnetic configurations and corresponding energy band structures. (a) and (b) for nanoribbon ZA, and (c) and (d) for nanoribbon AA. Magenta and cyan denote the  $\alpha$ - and  $\beta$ -spin components, respectively. The values for the  $\alpha$ - and  $\beta$ -spin isosurfaces are  $\pm 0.005 \text{ |e|/\AA}^3$

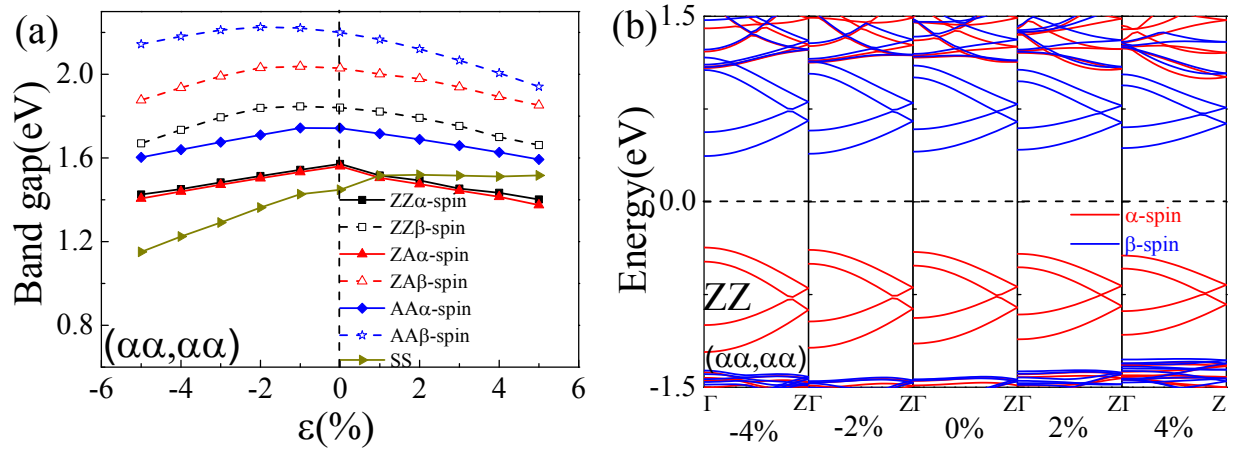


Fig.S3. (a) Effects of longitudinal strains on band gaps in various P-GNRs. (b) Evolution of the energy band structure with longitudinal strains for the nanoribbon ZZ

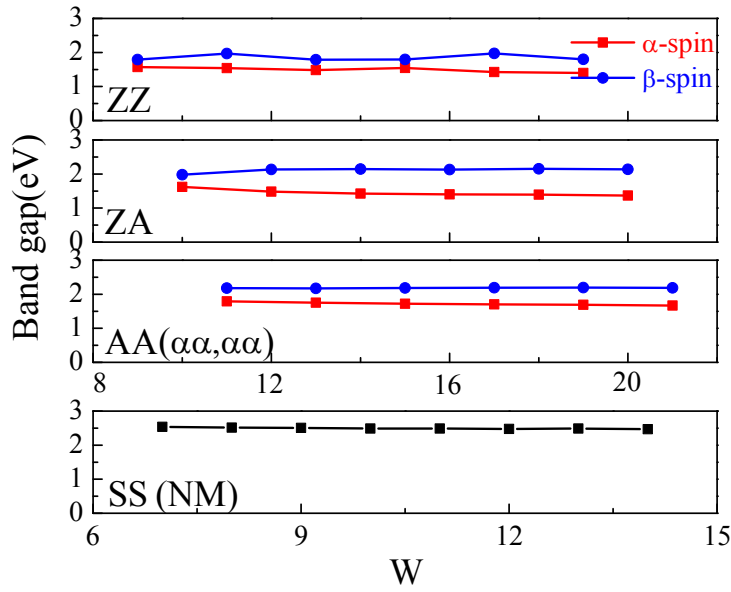


Fig.S4 Change of the band gap as a function of the ribbon width, where nanoribbons ZZ, ZA, and AA are supposed in the magnetic configuration  $(\alpha\alpha, \alpha\alpha)$ , and the nanoribbon SS is in the nonmagnetic state.