Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Coupling effects of electric field and bending on the electronic and magnetic properties of penta-graphene nanoribbons

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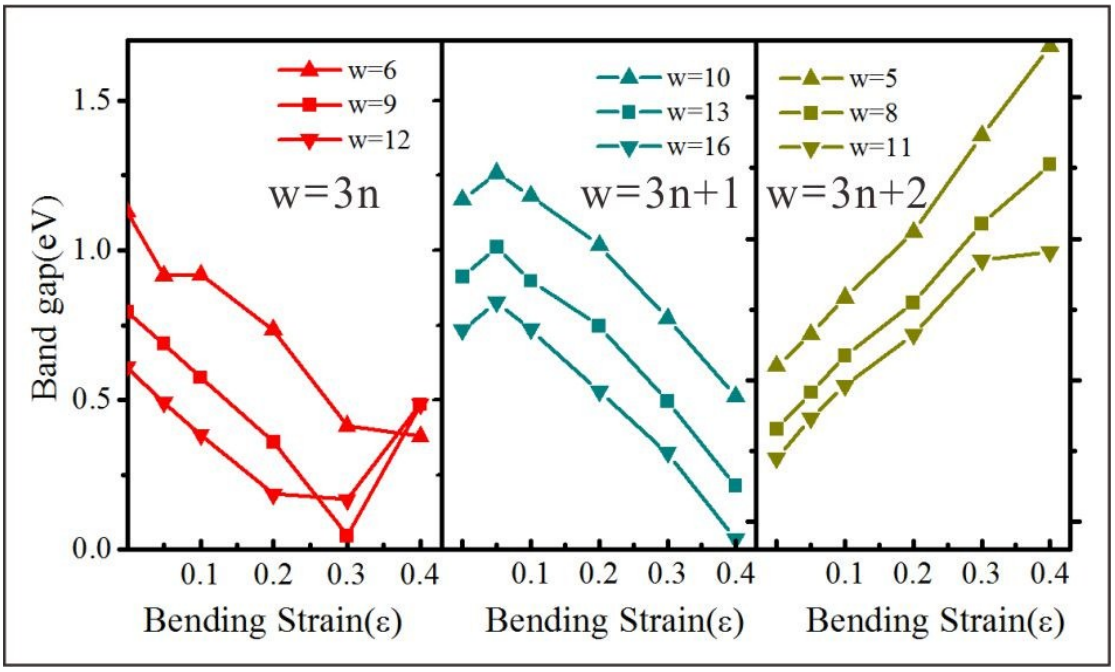

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Figure S1. The band gap variation for armchair GNRs under bending. Red, green, orange corresponds to width categories of 3n, 3n+1, 3n+2. Different width among the same category is denoted by different symbols.

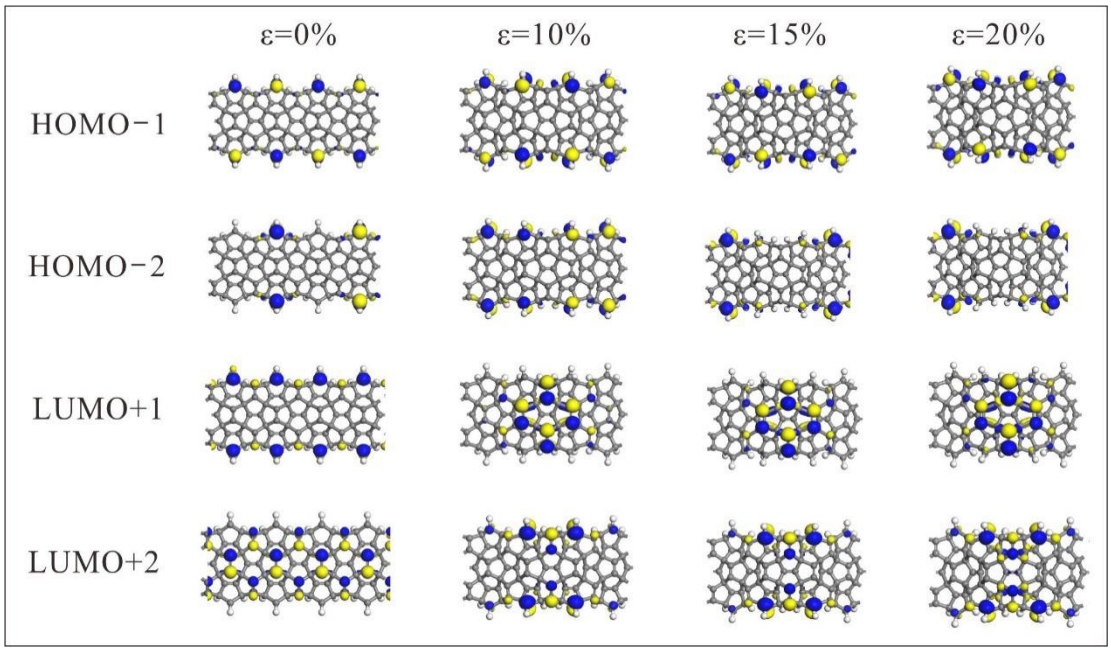

Figure S2. Charge densities of HOMO-1, HOMO-2, LUMO+1, LUMO+2 at the Gamma point for P-GNRs under bending strain of 0%, 10%, 15%, and 20%, respectively. Blue and yellow denote positive and negative wave function contours, respectively. The isosurface value is set to be ±0.02 e/Å^3.

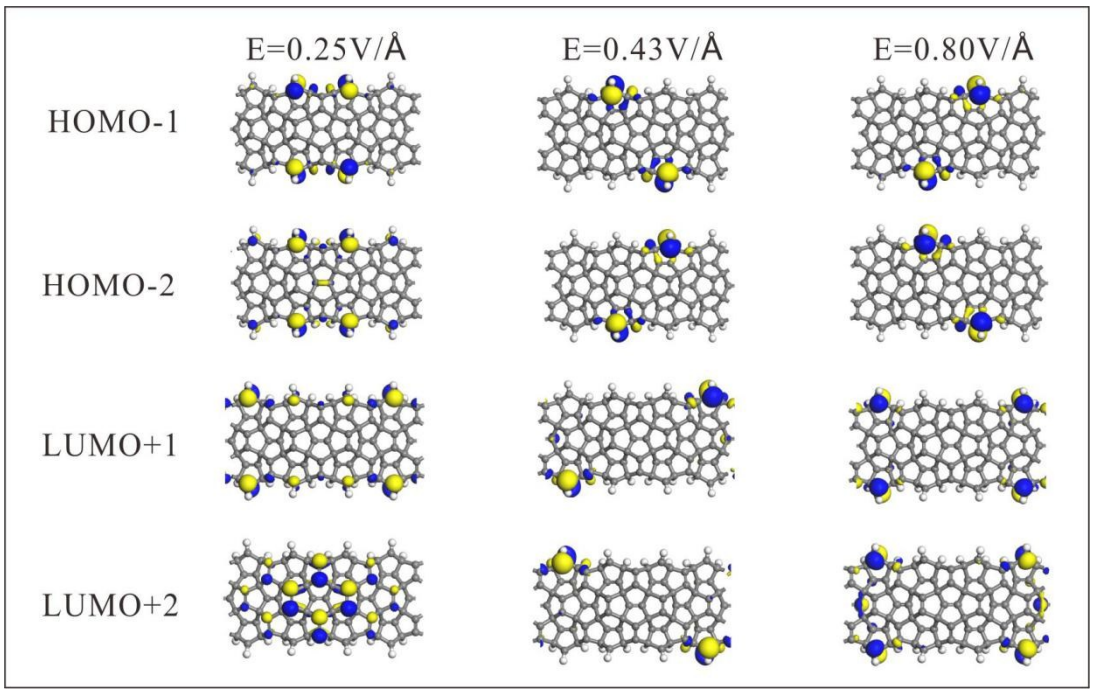

Figure S3. Charge densities of HOMO-1, HOMO-2, LUMO+1 and LUMO+2 at the Gamma point for bending P-GNRs (ε=10%) with electric field (E) 0.25V/Å, 0.43V/Å, and 0.80V/Å, respectively. Blue and yellow denote positive and negative wave function contours, respectively. The isosurface value is set to be ±0.02 e/Å^3.