

Supporting Information

Adsorption of Rare Base-pairs on Surface of B/N Atom Doped γ -graphyne from First Principles

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Fig. S1 Optimized configurations of the rare base-pairs on the B/N-doped on γ -GY nanosheet. (G-5-meCyt; G-5-hmCyt; G-5-caCyt; G-5-fCyt) Note that same color represents each atom is used for all of the graphics throughout the article.

Fig. S2 The CDD plots (isosurface value is $0.0003e/\text{\AA}$) of the base-pairs and rare base-pairs on the B-doped γ -GY nanosheet. (a: G-Cyt absorbed on B-doped γ -GY; b: G-5-meCyt absorbed on B-doped γ -GY; c: G-5-hmCyt absorbed on B-doped γ -GY; d: G-5-caCyt absorbed on B-doped γ -GY; e: G-5-fCyt absorbed on B-doped γ -GY).

Fig. S3 The CDD plots (isosurface value is $0.0003e/\text{\AA}$) of the base-pairs and rare base-pairs on the N-doped γ -GY nanosheet. (a: G-Cyt absorbed on N-doped γ -GY; b: G-5-meCyt absorbed on N-doped γ -GY; c: G-5-hmCyt absorbed on N-doped γ -GY; d: G-5-caCyt absorbed on N-doped γ -GY; e: G-5-fCyt absorbed on N-doped γ -GY).

Fig. S4 The Band structures of B-doped γ -GY and rare base-pairs on B-doped γ -GY nanosheet. (a: pure B-doped γ -GY; b: G-5-meCyt absorbed on B-doped γ -GY; c: G-5-hmCyt absorbed on B-doped γ -GY; d: G-5-caCyt absorbed on B-doped γ -GY; e: G-5-fCyt absorbed on B-doped γ -GY)

Fig. S5 The PDOS of B-doped γ -GY, base-pairs and rare base-pairs on B-doped γ -GY nanosheet (a: pure B-doped γ -GY; b: G-Cyt absorbed on B-doped γ -GY; c: G-5-meCyt absorbed on B-doped γ -GY; d: G-5-hmCyt absorbed on B-doped γ -GY; e: G-5-caCyt absorbed on B-doped γ -GY; f: G-5-fCyt absorbed on B-doped γ -GY).

Fig. S6 The Band structures of N-doped γ -GY, base-pairs and rare base-pairs on N-doped γ -GY nanosheet. (a: pure N-doped γ -GY; b: G-5-meCyt absorbed on N-doped γ -GY; c: G-5-hmCyt absorbed on N-doped γ -GY; d: G-5-caCyt absorbed on N-doped γ -GY; e: G-5-fCyt absorbed on N-doped γ -GY)

Fig. S7 The PDOS of N-doped γ -GY, base-pairs and rare base-pairs on N-doped γ -GY nanosheet. (a: pure N-doped γ -GY; b: G-Cyt absorbed on N-doped γ -GY; c: G-5-meCyt absorbed on N-doped γ -GY; d: G-5-hmCyt absorbed on N-doped γ -GY; e: G-5-caCyt absorbed on N-doped γ -GY; f: G-5-fCyt absorbed on N-doped γ -GY).

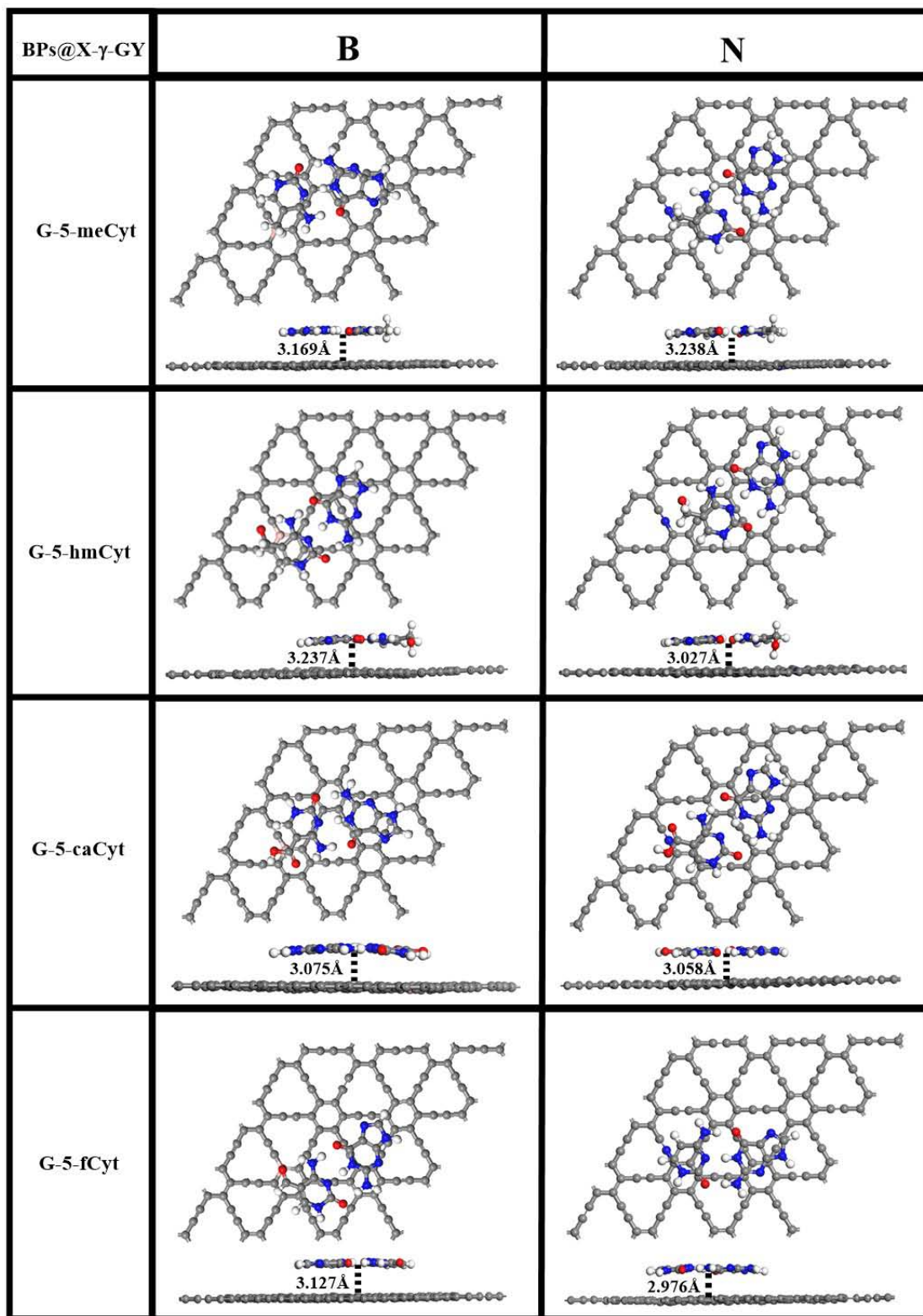


Fig. S1

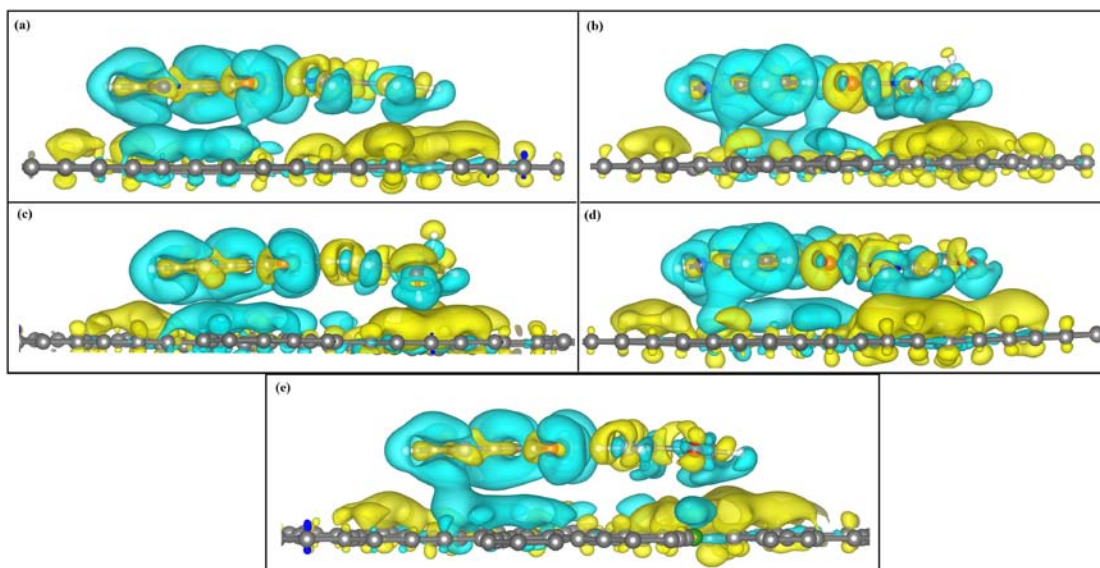


Fig. S2

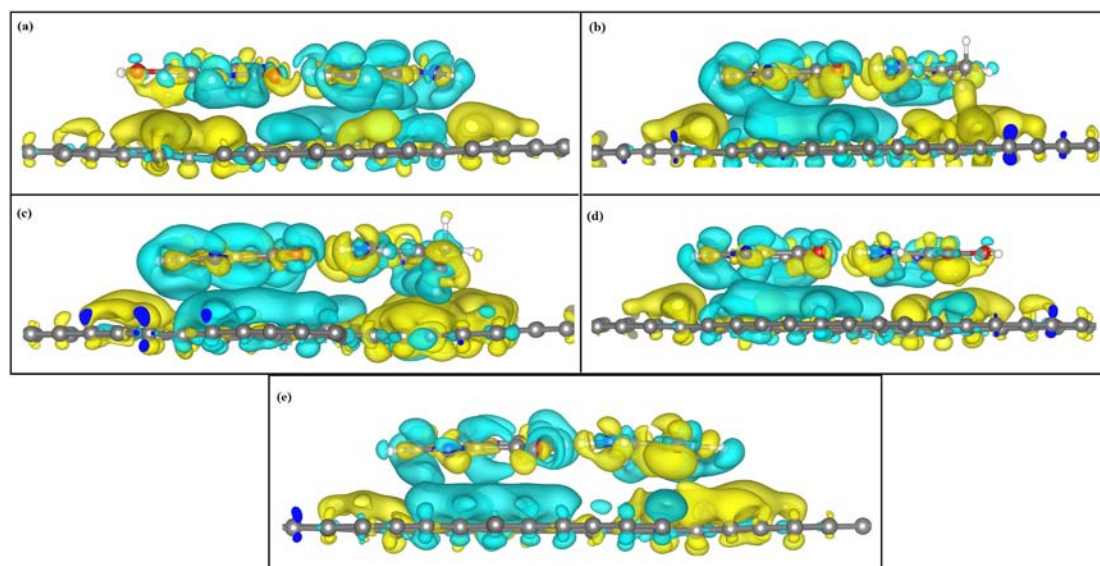


Fig. S3

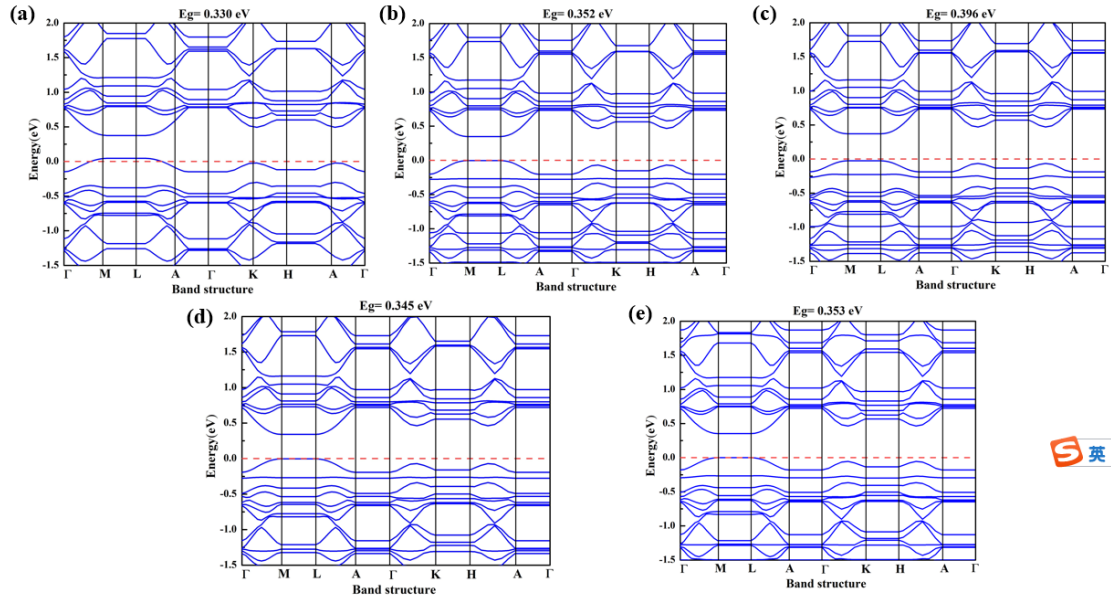


Fig. S4

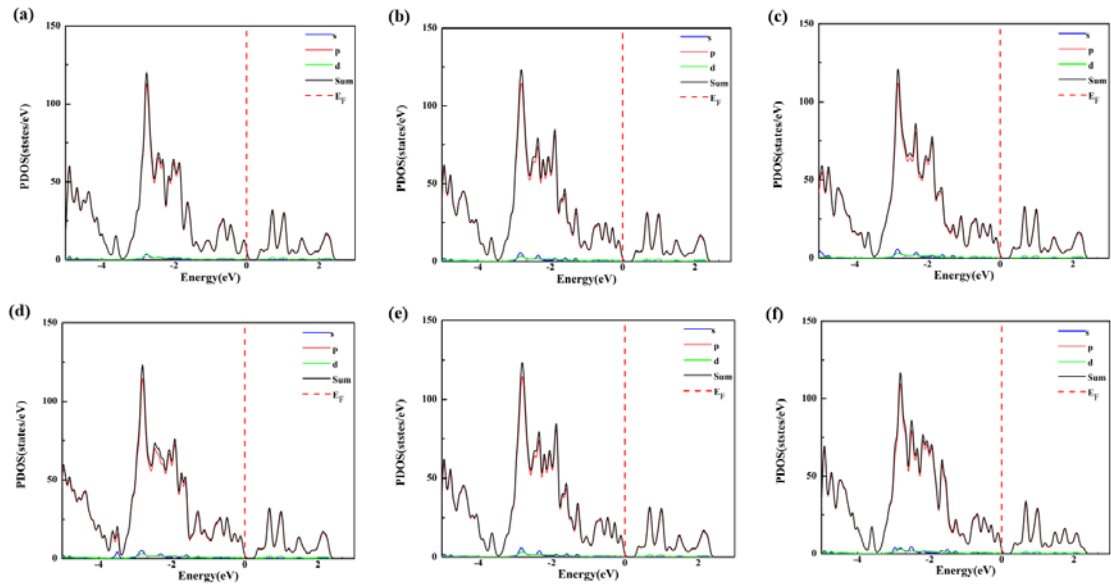


Fig. S5

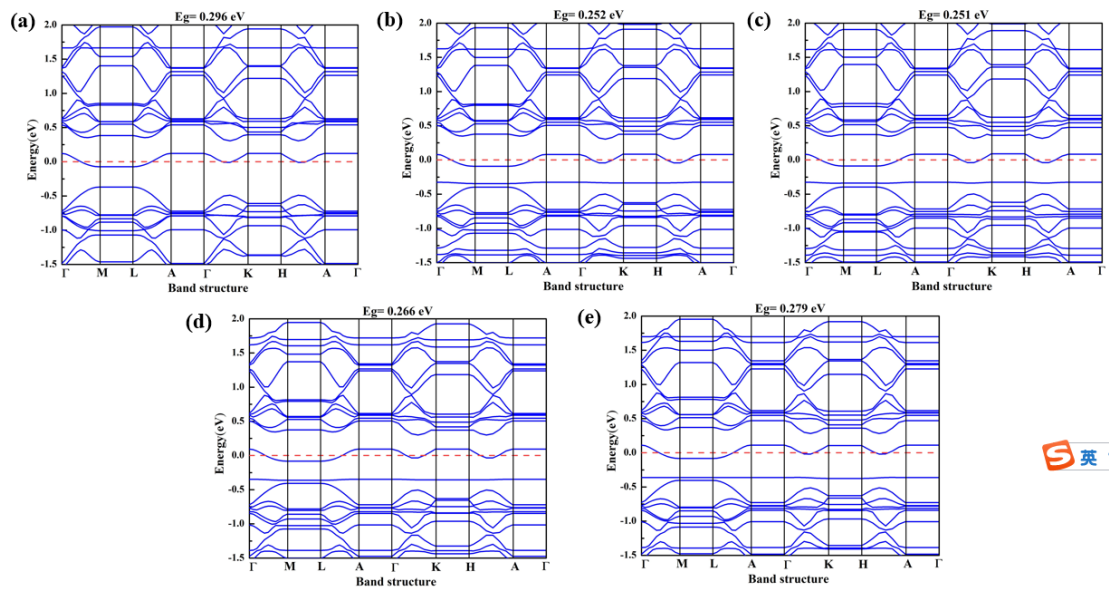


Fig. S6

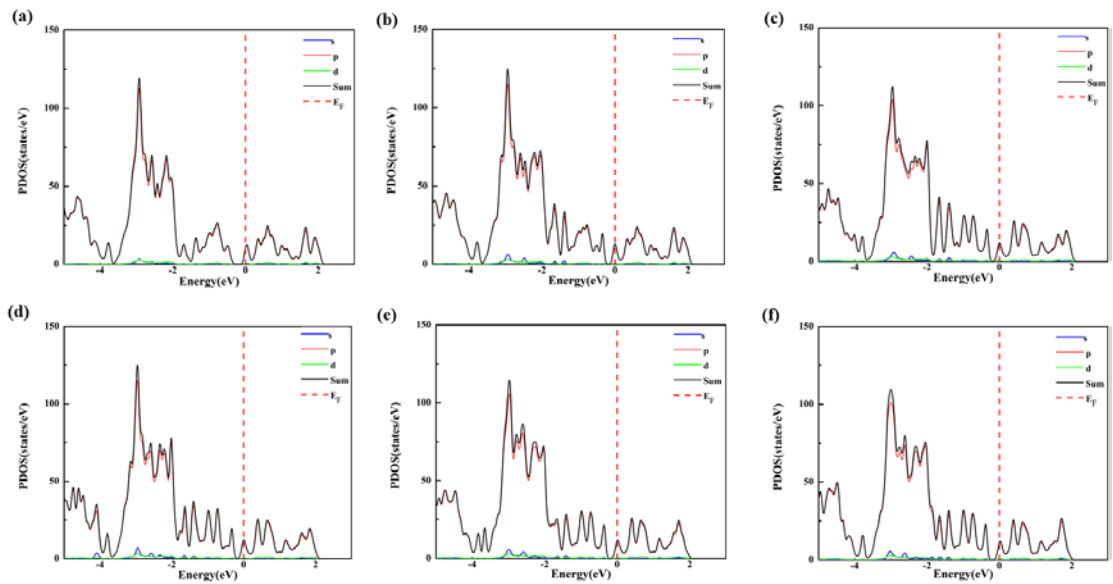


Fig. S7