Supplementary Materials

Ab-Initio Study of the Electronic and Magnetic Properties of Boron- and Nitrogen-Doped Penta-Graphene

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Figure S1. Atomic net magnetic moments (μ _B) for the (**a**) PG–B (sp²), (**b**) PG–B (sp³), (**c**) PG–N (sp²) and (**d**) PG–N (sp³) systems. Gray, pink and blue balls represent the carbon, boron, and nitrogen atoms, respectively.



Figure S2. Atomic hirshfeld charge (|e|) for the (**a**) PG–B (sp²), (**b**) PG–B (sp³), (**c**) PG–N (sp²) and (**d**) PG–N (sp³) systems. Gray, pink and blue balls represent the carbon, boron, and nitrogen atoms, respectively.



Figure S3. Bond lengths (Å) for the (**a**) PG–B (sp²), (**b**) PG–B (sp³), (**c**) PG–N (sp²) and (**d**) PG–N (sp³) systems. Gray, pink and blue balls represent the carbon, boron, and nitrogen atoms, respectively.