Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

Applying the Surface Strain and Coupling with Pure or N/B-Doped Graphene to Successfully Achieve the High HER Catalytic Activity in the 2D Layered SnP_3-Based Nanomaterials: A First-Principle Investigation

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(I) The computational test on adopting the stacking mode for the few-layered SnP_3 nanostructures

For the 2D few-layered SnP_3 nanostructures, we adopt the similar stacking model to the bulk structure, which belongs to the AB stacking model that each Sn/P atom on the upper layer is located over the center of each hexagonal ring of lower layer (Figure 2). Here, to evaluate relative stability, we also consider other possible configurations (II-V) with AB stacking as well as the possible configurations (VI) with AA stacking model with a hexagonal stacking arrangement by sampling bilayer SnP_3 systems (Figure S1). The computed results reveal that the bilayer configuration (I) with the similar AB stacking to the bulk structure can be energetically lowest-lying one among all these configurations (Figure S1), indicating the highest structural stability. Thus, the similar AB stacking model to the bulk structure has been adopted for all the few-layered SnP_3 systems in this study.

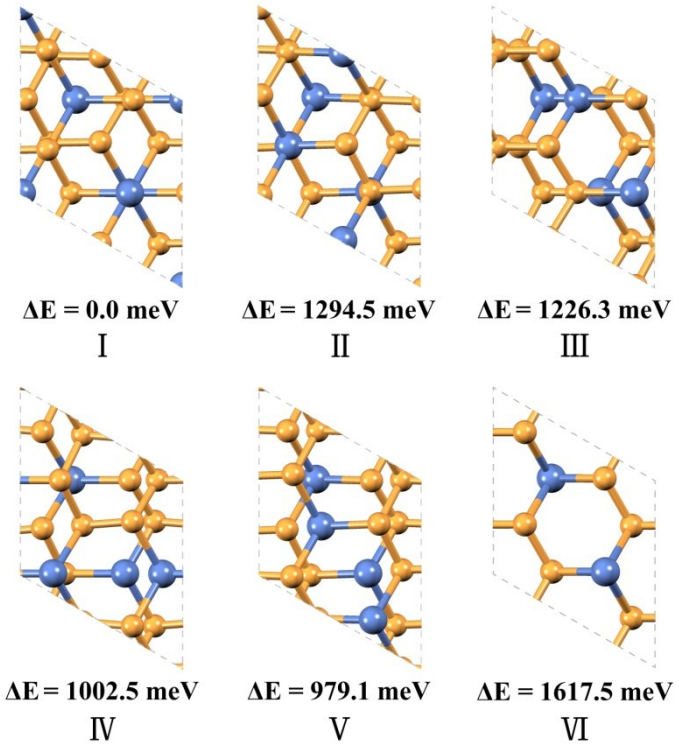

Figure S1 The top views of 2L-SnP_3 systems with different configurations and their relative energies.

(II) The relative energies of doped 2L-SnP_3/G nanostructures with N or B atom at the different sites

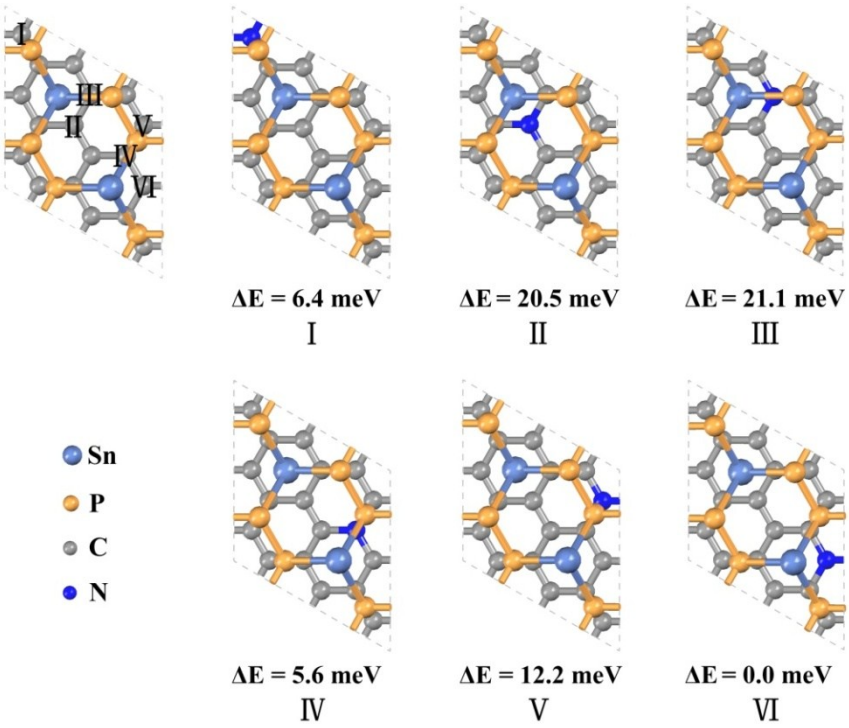

Figure S2 The top views of 2L-SnP_3/NG systems with N-doping at different sites (I~VI) and their relative energies.

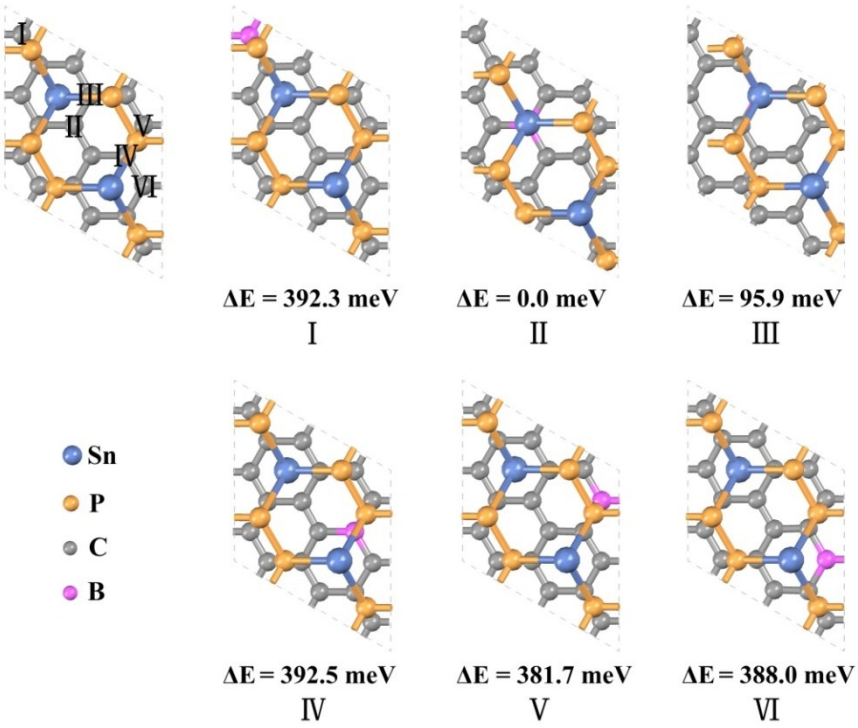

Figure S3 The top views of 2L-SnP_3/BG systems with B-doping at different sites (I~VI) and their relative energies.