Supporting Information

Exploring the Emerging of Electronic and Magnetic Properties with Adatom Adsorption on Novel Semiconduction Monolayer: N_2P_6

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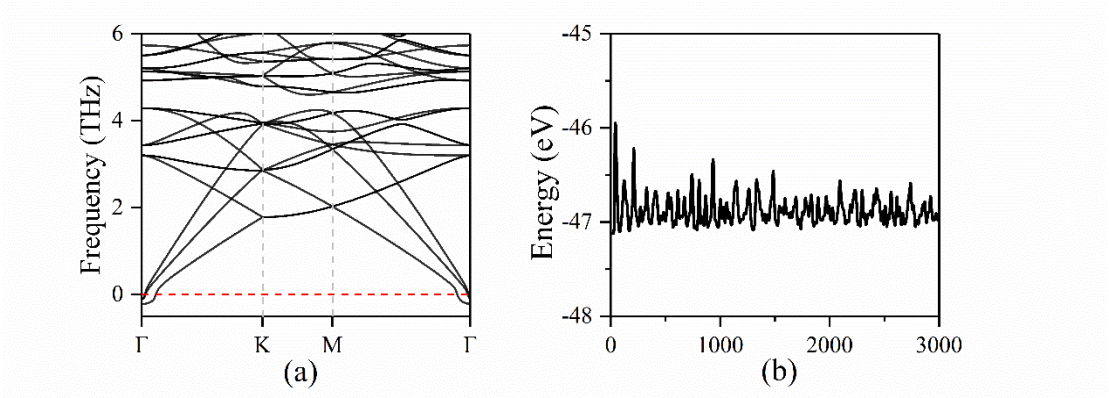

Figure S1. (a) The calculated phonon spectrum of N_2P_6 monolayer. (b) The evolution of total energies on N_2P_6 monolayer during FPMD simulation at 300 K.

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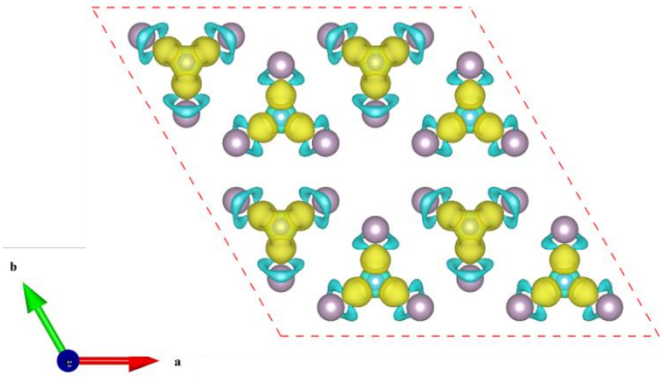

Figure S2. The top view of difference charge density with pristine N_2P_6 (isosurfaces = 0.01 $e(Å^3)^{-1}$). Brown dots are *P* atoms, and others are *N* atoms.

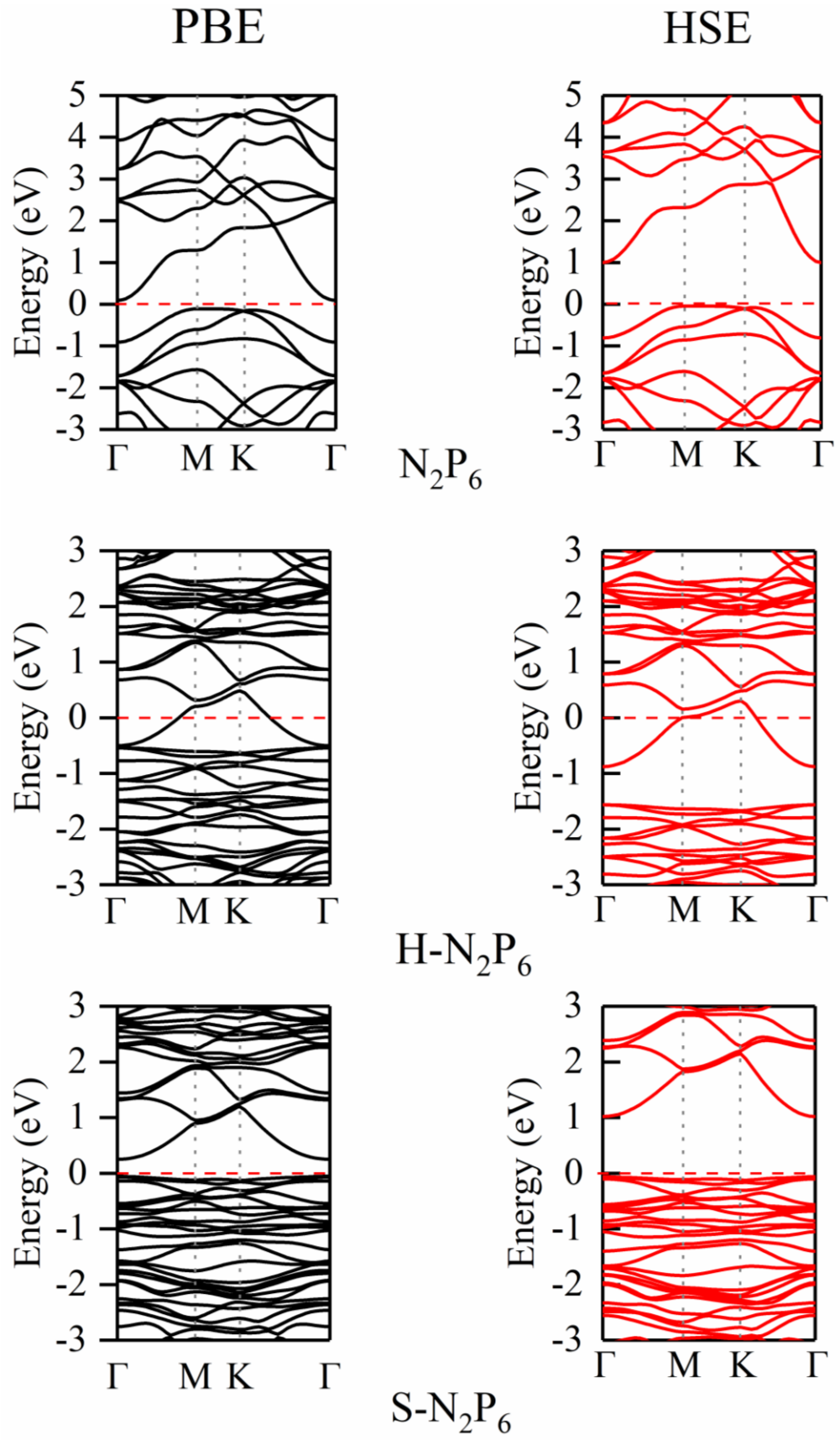

Figure S3: The band structures of three monolayers: (a)N_2P_6, (b) H-N_2P_6 and (c) S-N_2P_6 using PBE (left panel) and HSE06 (right panel), respectively. The Fermi level is set at 0 eV.

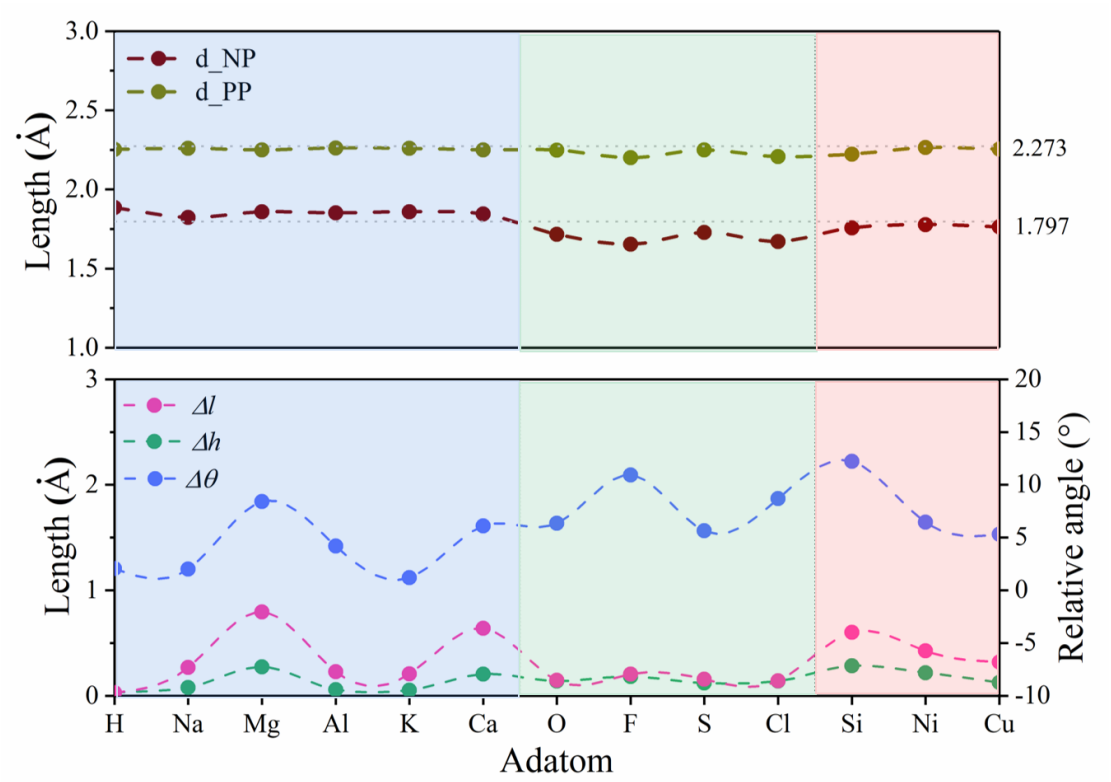

Figure S4. Variation of structural parameters for different adatoms adsorbed on N_2P_6 at the TN (light bule area), T_P (light green area), H_{PP} (light red area) sites. Δl ($\Delta l=lp\text{-}p\text{-}lp\text{-}p_{(sub0)}$) is used to describe in-plane distortion, and out-plane distortion is described by Δh ($\Delta h=h\text{-}h_{sub0}$). Relative angle ($\Delta\theta=\theta\text{-}\theta_0$, θ_0=88.889º) is defined as the maximum variation of angle θ made up by adatoms nearest P atom and its first and second bond length of P-P.

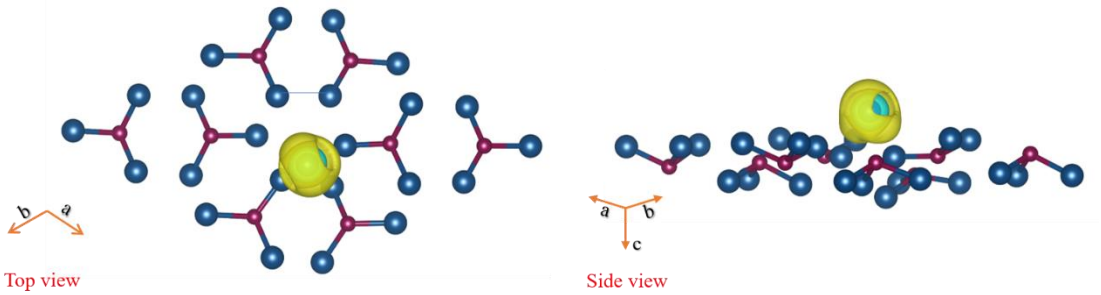

Figure S5. The top view and side view of difference charge density for P adatom adsorbed on pristine N_2P_6 (isosurfaces = 0.02 e(Å^3)$^{-1}$). Brown dots are P atoms, and others are N atoms.