Supporting Information

Exploring the Emerging of Electronic and Magnetic Properties with Adatom Adsorption on Novel Semiconduction Monolayer: N$_2$P$_6$

Xinle Lu$^{1,2}$, Liao­xin Sun$^2$, Bing Fu$^3$, Shoutian Sun$^1$* and Xiang Ye$^1$*

$^1$Department of Physics, Shanghai Normal University, Shanghai 200234, P. R. China
$^2$State Key Laboratory of Infrared Physics, Chinese Academy of Sciences, Shanghai 200083, P. R. China
$^3$Fuzhou Medical College of Nanchang University, Fuzhou 344000, P. R. China

Corresponding Author: stsun@shnu.edu.cn (Shoutian Sun), yexiang@shnu.edu.cn (Xiang Ye)

Figure S1. (a) The calculated phonon spectrum of N$_2$P$_6$ monolayer. (b) The evolution of total energies on N$_2$P$_6$ monolayer during FPMD simulation at 300 K.

* Email address: stsun@shnu.edu.cn (Shoutian Sun), yexiang@shnu.edu.cn (Xiang Ye)
Figure S2. The top view of difference charge density with pristine N\textsubscript{2}P\textsubscript{6} (isosurfaces = 0.01 e(\textsubscript{\text{Å}}\textsuperscript{3})\textsuperscript{-1}). Brown dots are P atoms, and others are N atoms.
Figure S3: The band structures of three monolayers: (a) N$_2$P$_6$, (b) H-N$_2$P$_6$, and (c) S-N$_2$P$_6$ 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$_2$P$_6$ at the TN (light blue area), T$_P$ (light green area), H$_{PP}$ (light red area) sites. $\Delta l$ (\(\Delta l=lp-lp_{(sub)}\)) is used to describe in-plane distortion, and out-plane distortion is described by $\Delta h$ (\(\Delta h=h-h_{(sub)}\)). Relative angle ($\Delta \theta=\theta-\theta_0$, \(\theta_0=88.889^\circ\)) is defined as the maximum variation of angle $\theta$ 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.