Electronic Supplementary Information

A First-principles study on the magnetic properties of nonmetal atoms doped monolayer phosphorene

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S1. MD snapshots of P_{143}X(X=H, F, Cl, Br, I, B, N, As, Si, O, S, and Se) at 300K.

S2. MD movies of P_{143}X(X=H, F, Cl, Br, I, B, N, As, Si, O, S, and Se) at 300K.

S3. Calculated formation energies as a function of Fermi level for the substitutional dopants in monolayer phosphorene.

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Figure S1. MD snapshots of P$_{143}$X (X=H, F, Cl, Br, I, B, N, As, C, Si, O, S and Se) at 300K.

(a)P$_{143}$H:t=0ps         (b)P$_{143}$H:t=0.75ps        (c)P$_{143}$H:t=1.5ps

(d)P$_{143}$F:t=0ps          (e)P$_{143}$F:t=0.75ps         (f)P$_{143}$F:t=1.5ps

(g)P$_{143}$Cl:t=0ps         (h)P$_{143}$Cl:t=0.75ps        (i)P$_{143}$Cl:t=1.5ps

(j)P$_{143}$Br:t=0ps         (k)P$_{143}$Br:t=0.75ps        (l)P$_{143}$Br:t=1.5ps

(m)P$_{143}$I:t=0ps          (n)P$_{143}$I:t=0.75ps         (o)P$_{143}$I:t=1.5ps

Figure S1. MD snapshots of P$_{143}$X(X=H, F, Cl, Br and I). Lavender and pink balls represent P and doping X atoms, respectively.
Figure S2. MD snapshots of $P_{143}X$ ($X=B$, N and As). Lavender and pink balls represent P and doping X atoms, respectively.
Figure S3. MD snapshots of P$_{143}$X (X=C, Si, O, S and Se). Lavender and pink balls represent P and doping X atoms, respectively.
S2. MD movies of $P_{143}X$($X$=H, F, Cl, Br, I, B, N, As, C, Si, O, S, and Se) at 300K.

- H-doped-300K.wmv represents the $P_{143}H$ at $T$=300K.
- F-doped-300K.wmv represents the $P_{143}F$ at $T$=300K.
- Cl-doped-300K.wmv represents the $P_{143}Cl$ at $T$=300K.
- Br-doped-300K.wmv represents the $P_{143}Br$ at $T$=300K.
- I-doped-300K.wmv represents the $P_{143}I$ at $T$=300K.
- B-doped-300K.wmv represents the $P_{143}B$ at $T$=300K.
- N-doped-300K.wmv represents the $P_{143}N$ at $T$=300K.
- As-doped-300K.wmv represents the $P_{143}As$ at $T$=300K.
- C-doped-300K.wmv represents the $P_{143}C$ at $T$=300K.
- Si-doped-300K.wmv represents the $P_{143}Si$ at $T$=300K.
- O-doped-300K.wmv represents the $P_{143}O$ at $T$=300K.
- S-doped-300K.wmv represents the $P_{143}S$ at $T$=300K.
- Se-doped-300K.wmv represents the $P_{143}Se$ at $T$=300K.
S3. Calculated formation energies as a function of Fermi level for the substitutional dopants in monolayer phosphorene.

Figure S4. Calculated formation energies as a function of the Fermi level for (a) H and H$^{4-}$, (b) F and F$^{2+}$, (C) Cl and Cl$^{2+}$, (d) Br and Br$^{2+}$, (e) I and I$^{2+}$, (f) B and B$^{2-}$, (h) O and O$^+$ dopants in monolayer phosphorene. The zero of Fermi level corresponds to the valence-band maximum.
Figure S5. Calculated formation energies as a function of the Fermi level for (a) C and C−, (b) Si and Si−, (C) S and S+, (d) Se and Se+ dopants in monolayer phosphorene. The red dots represent the transition levels. The zero of Fermi level corresponds to the valence-band maximum.