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, C, Si, O, S, and Se) at 300K.

S2. MD movies of $P_{143}X$(X=H, F, Cl, Br, I, B, N, As, C, 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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S1. MD snapshots of $P_{143}X$ (X=H, F, Cl, Br, I, B, N, As, C, Si, O, S and Se) at 300K.

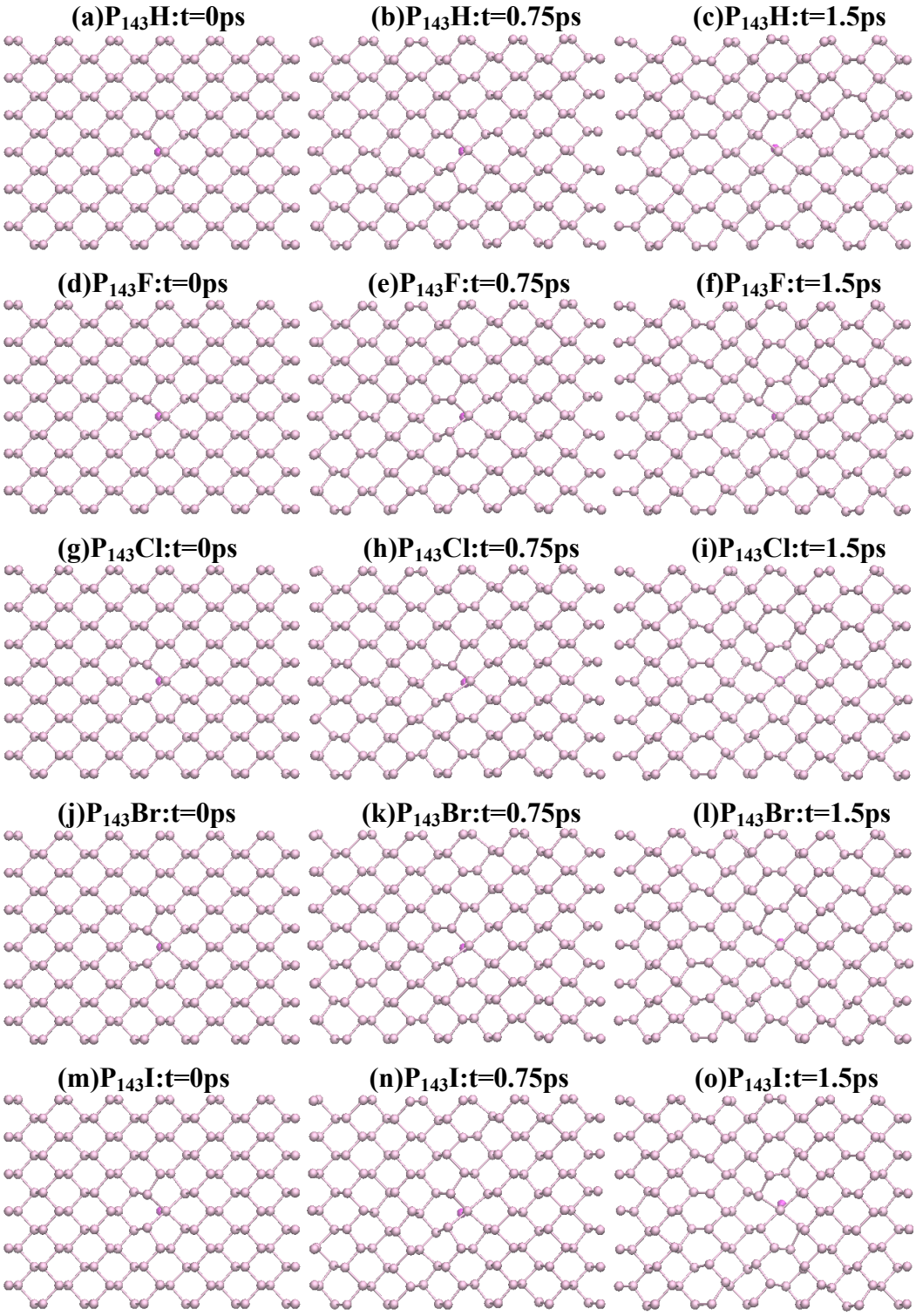

Figure S1. MD snapshots of $P_{143}X$(X=H, F, Cl, Br and I). Lavender and pink balls represent P and doping X atoms, respectively.

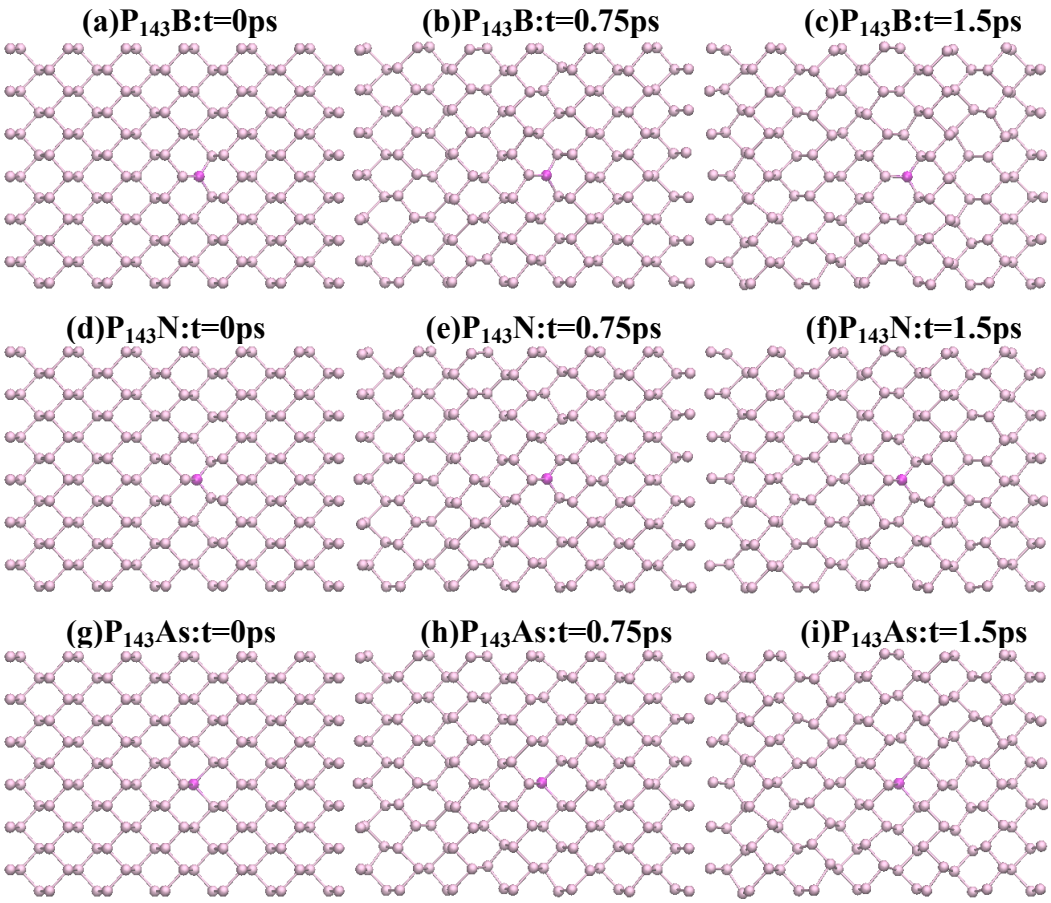

Figure S2. MD snapshots of $P_{143}X$(X=B, N and As). Lavender and pink balls represent P and doping X atoms, respectively.

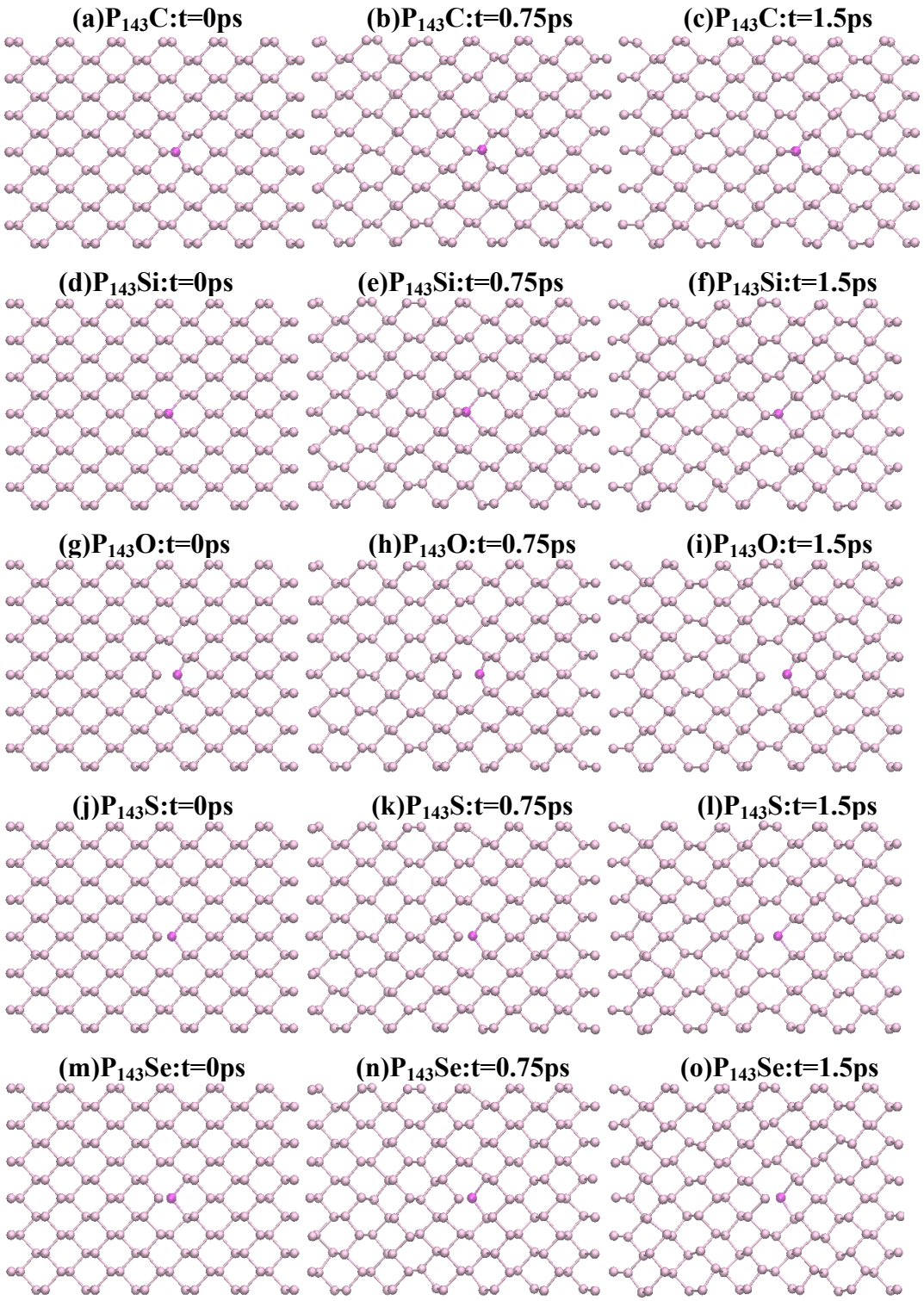

Figure S3. MD snapshots of $P_{143}X$(X=C, Si, O, S and Se). Lavender and pink balls represent P and doping X atoms, respectively.

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.

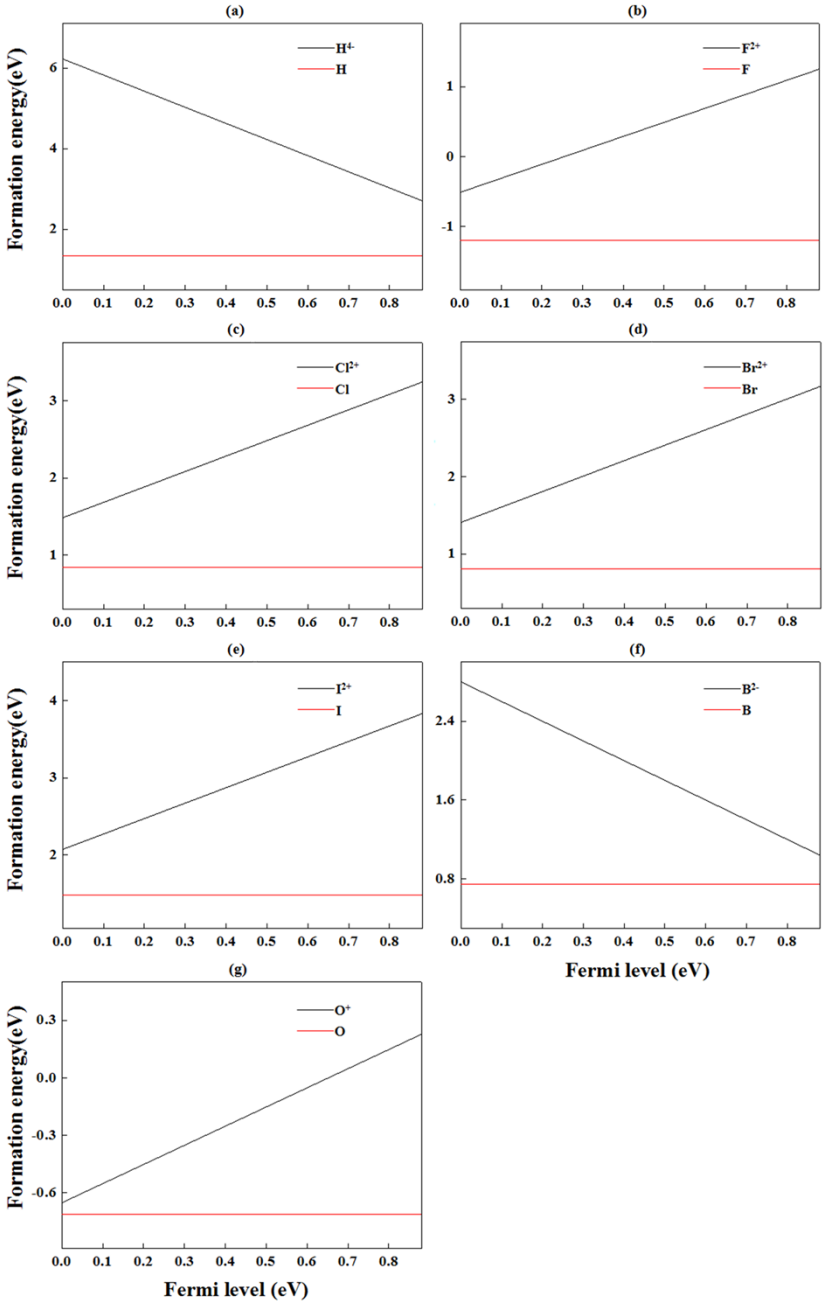

Figure S4. Calculated formation energies as a function of the Fermi level for (a) H and H^{4-}, (b) F and F^{2+}, (C) Cl and Cl^{2+}, (d) Br and Br^{2+}, (e) I and I^{2+}, (f) B and B^{2-}, (h) O and O^{+} dopants in monolayer phosphorene. The zero of Fermi level corresponds to the valence-band maximum.

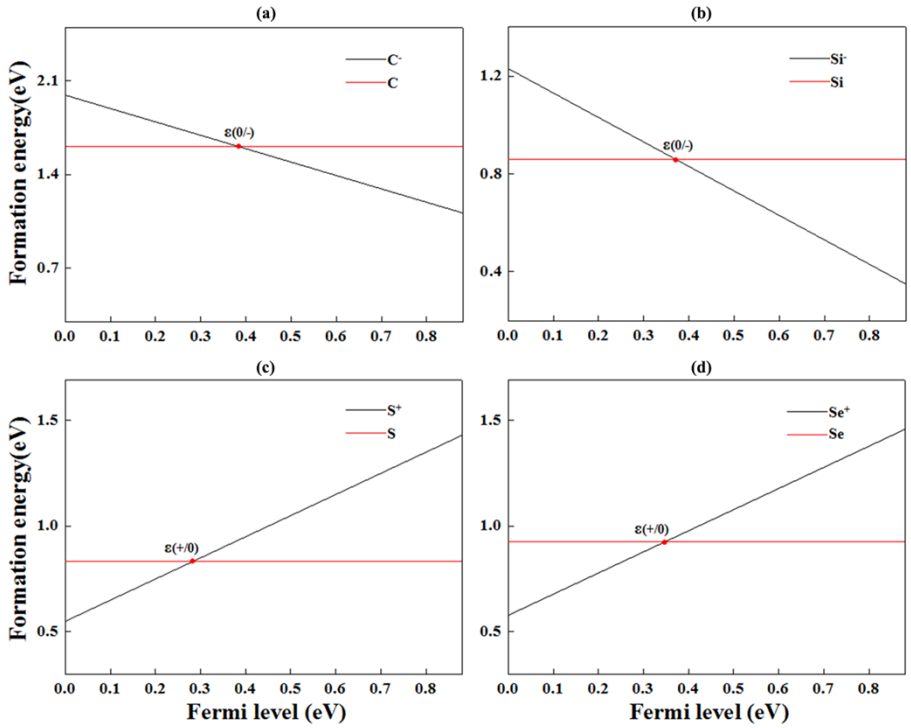

Figure S5. Calculated formation energies as a function of the Fermi level for (a) C and C^-, (b) Si and Si^-, (C) S and S^+, (d) Se and Se^+ dopants in monolayer phosphorene. The red dots represent the transition levels. The zero of Fermi level corresponds to the valence-band maximum.