Electronic Supplementary Information

Tuning the mechanical, electronic properties and carrier mobility of phosphorene via family atom doping: a first-principles study

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S1. Geometric structures of doped phosphorene

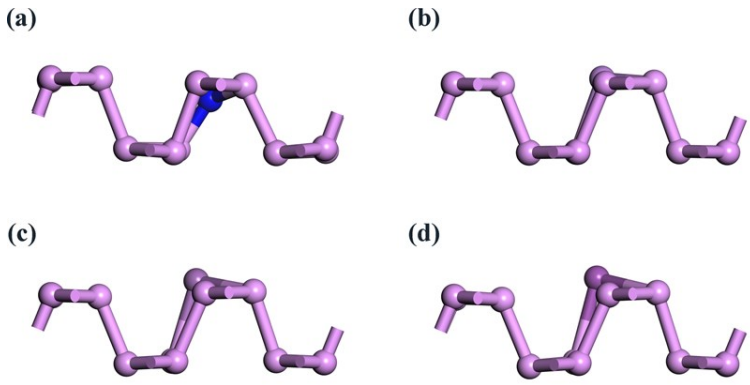

Fig. S1 Optimized geometric structures for the phosphorene supercell doped with (a) N, (b) As, (c) Sb, and (d) Bi atoms (side views). The pale magenta spheres represent the phosphorus atoms and other colors represent dopant atoms.

S2. Poisson's ratio of pure and doped phosphorene

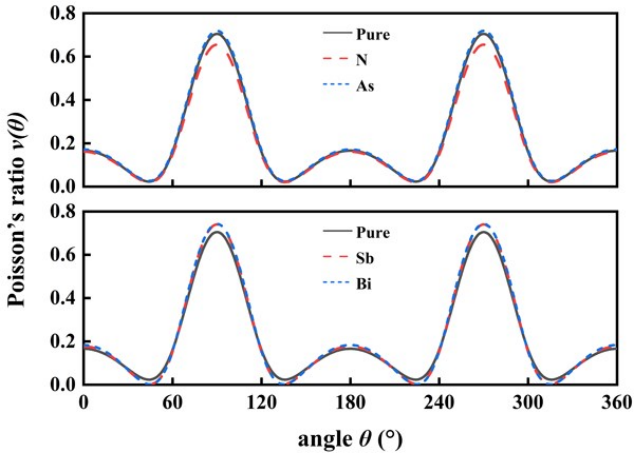

Fig. S2 Poisson's ratio $\nu(\theta)$ is expressed as a function of the angle θ for the pure and doped phosphorene. The graph is the form of Fig. 4(b) converted to Cartesian coordinate system.

S3. Band structure of N-doped phosphorene calculated by PBE method

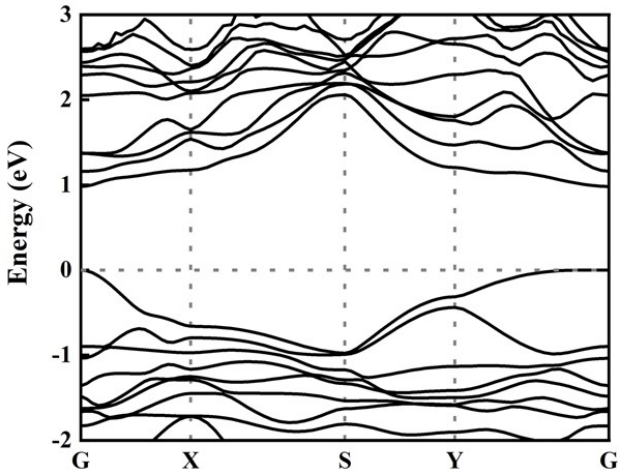

Fig. S3 Calculated band structure of N-doped phosphorene using PBE method. The CBM is located at G point, and the position of the VBM is slightly shifted from the G point. The value of the quasi-direct bandgap is 0.982 eV.

S4. Calculated band structure for 1 × 2 N-doped phosphorene supercell with HSE06 functional

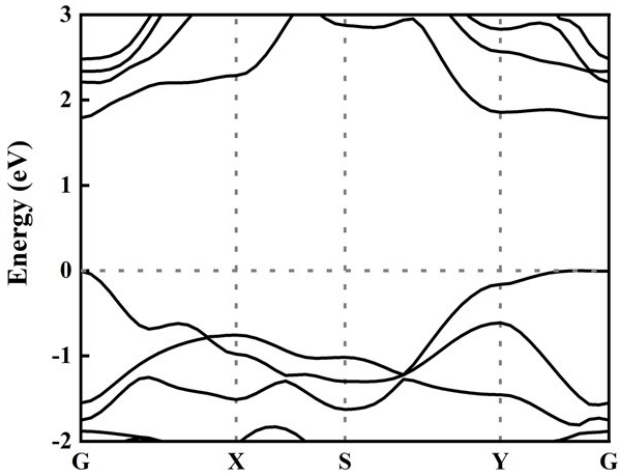

Fig. S4 Calculated band structure for 1 × 2 phosphorene supercell doped with one N atom using the HSE06 functional. The k-point mesh and path density is the same as that for 2 × 2 supercell calculations. The bandgap value is 1.790 eV.

S5. Calculated band structures of Sb and Bi doped phosphorene by HSE06 with SOC

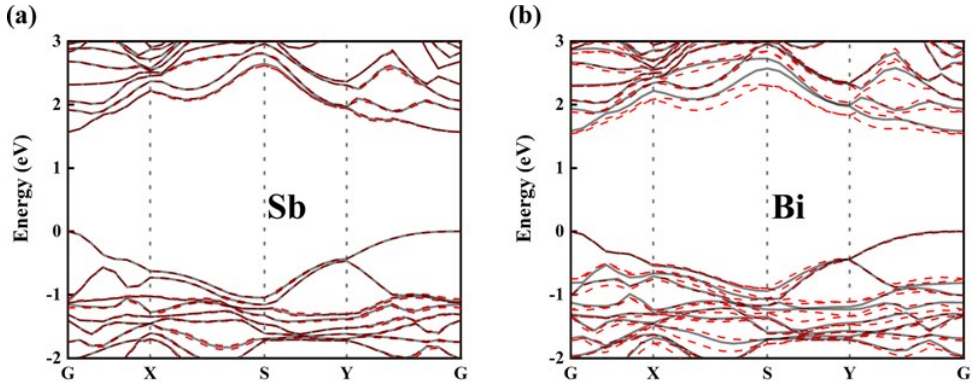

Fig. S5 SOC effects on the band structures of (a) Sb and (b) Bi doped phosphorene. The calculated band structures without SOC are draw with gray lines. The red lines are the results with SOC. The bandgap value is 1.566 eV (1.540 eV) for Sb-doped (Bi-doped) phosphorene with SOC.

S6. Carrier mobility calculated using the phono-limited scattering model

The phonon-limited scattering model to calculate the 2D carrier mobility:

$$\mu_x = \frac{e\hbar^3}{k_B T\left(m_x^*\right)^{3/2}\left(m_y^*\right)^{1/2}}\left(\frac{A+B-\sqrt{A^2-B^2}}{B\sqrt{A^2-B^2}}\right)\times\left(\frac{I+J-\sqrt{I^2-J^2}}{J\sqrt{I^2-J^2}}\right)$$

where the parameters A, B, I, and J are defined as

$$A = \overline{E}_1{}^2 + \frac{\Delta E_1{}^2}{2}, \quad B = \overline{E}_1 \Delta E_1$$

$$I = \frac{1}{\sqrt{\overline{C}^2 - \Delta C^2}}, \quad J = \frac{\overline{C}}{\Delta C}\left(\frac{1}{\overline{C}} - \frac{1}{\sqrt{\overline{C}^2 - \Delta C^2}}\right)$$

where $\overline{E}_1$, ΔE, $\overline{C}$, and ΔC denote the averages and differences in the deformation potential and elastic constants along the x and y directions:

$$\overline{E}_1 = \frac{E_{1y} + E_{1x}}{2}, \quad \Delta E = \frac{E_{1y} - E_{1x}}{2}$$

$$\overline{C} = \frac{C_y + C_x}{2}, \quad \Delta C = \frac{C_y - C_x}{2}$$

The calculated results using this model are listed in Table S1. The mobility anisotropy is mainly contributed by the anisotropic effective mass, while the contribution from the deformation potential and elastic constants are much weaker. The electron mobility and hole mobility along the *x*-direction are higher than those along the *y*-direction for all systems. The electron mobility is little changed and the hole mobility is improved by the As, Sb, and Bi doping. Although different from the results obtained by the old formula, the conclusion that N doping increases both electron mobility and hole mobility is consistent.

Table S1 Calculated carrier mobility (μ, 10^3 $cm^2V^{-1}s^{-1}$) using the phono-limited scattering model along *x* (armchair) and *y* (zigzag) directions at T = 300K temperature.

Carrier type	System	m_x^*/m_0	m_y^*/m_0	E_{1x}	E_{1y}	C_{x_2D}	C_{y_2D}	μ_{x_2D}	μ_{y_2D}
e	Pure	0.207	1.120	1.53	5.19	24.67	104.66	1.04	0.17
	N	0.449	1.063	0.74	2.33	25.61	104.21	1.63	0.60
	As	0.212	1.115	1.51	5.23	24.05	100.81	0.97	0.16
	Sb	0.227	1.068	1.23	4.9	22.33	93.44	1.02	0.18
	Bi	0.236	1.090	1.04	4.6	21.79	88.33	1.09	0.19
h	Pure	0.186	8.176	2.77	0.12	24.67	104.66	1.16	0.08
	N	0.228	3.591	2.52	0.15	25.61	104.21	1.57	0.30
	As	0.190	5.300	2.79	0.15	24.05	100.81	1.32	0.14
	Sb	0.200	4.999	2.54	0.21	22.33	93.44	1.38	0.16
	Bi	0.219	5.357	2.38	0.19	21.79	88.33	1.28	0.15

The carrier types 'e' and 'h' represent electron and hole, respectively. The effective masses m_x^* and m_y^* are labeled by m_0. The deformation potential is given using E_1 (eV). The unit of elastic modulus C_{2D} is N/m.