Supplementary Materials

Phonon-mediated superconductivity in two-dimensional hydrogenated phosphorus carbide: HPC$_3$

Ya-Ping Li$^1$, Liu Yang$^1$, Hao-Dong Liu$^1$, Na Jiao$^1$, Mei-Yan Ni$^1$, Ning Hao$^2$, Hong-Yan Lu$^{1,*}$, and Ping Zhang$^{1,3,*}$

$^1$School of Physics and Physical Engineering, Qufu Normal University, Qufu 273165, China
$^2$Anhui Province Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory, HFIPS, Chinese Academy of Sciences, Hefei 230031, China
$^3$Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

Corresponding Authors
*E-mail:(H. Y. L.) hylu@qfnu.edu.cn
*E-mail:(P. Z.) pzhang2012@qq.com
I. The electronic band structure and DOS of PC$_3$

We calculated the electronic band structure and DOS of the monolayer PC$_3$ based on first principles calculations, with the results shown in the Fig. S1. Fig. S1(a) shows the electronic band structure of PC$_3$. There are no bands crossing the Fermi level and an indirect bandgap of 1.488 eV is seen, proving that the monolayer PC$_3$ is a semiconductor. Fig. S1 is the total DOS and the total DOS of each element. These results are consistent with the band structure, DOS and bandgap given in the previous literature [1].

![Electronic band structure and DOS](image)

FIG. S1: (a) The electronic band structure of PC$_3$ along high-symmetry line Γ-M-K-Γ. (b) The total DOS of PC$_3$ and total DOS of P and C atoms.

II. The vibration modes of HPC$_3$ at Γ point

Since there are ten atoms in the unit cell, there are thirty vibration modes for HPC$_3$. The modes at Γ point are shown in Fig. S2. Fig. S2 (1-3) shows the acoustic phonon modes at zero frequency. It shows the characteristic of typical acoustic mode vibration, i.e., all atoms vibrate in the same direction. The rests of vibration modes are optical phonon modes, revealing the relative vibrations of H, P, and C atoms. In the range $0 < \omega < 434$ cm$^{-1}$, the out-of-plane vibration of C atoms is the main contribution, and the vibration contribution of H atoms and P atoms is small. In the range $434 < \omega < 1352$ cm$^{-1}$, the in-plane modes of C atoms and the in-plane vibration of H atoms are the main contribution. At 2130 cm$^{-1}$, the out-of-plane vibration of H is the main contribution. Above results are consistent with those shown Fig. 3(b). More information about the vibration modes at Γ point, including the symmetry, vibration, Raman/infrared activity and frequencies are listed in Table S1, which provides a theoretical basis for future experimental verification.
FIG. S2: The thirty vibration modes of pristine HPC$_3$ at $\Gamma$ point in the Brillouin zone. The vibration frequencies are shown below each figure. The yellow, green, and blue spheres represent phosphorus, carbon, and hydrogen atoms, respectively, and the red arrow represents the direction of atomic vibration.

TABLE S1: The symmetry, vibration, activity (I and R represent infrared and Raman activity, respectively) and frequency (in cm$^{-1}$) for the thirty vibration modes at $\Gamma$ point.

| Modes | Symmetry | Vibration | Activity | Freq. (cm$^{-1}$) |
|-------|----------|-----------|----------|------------------|
| 1-2   | E        | Translational | I+R      | 0                |
| 3     | A.1      | Translational | I+R      | 0                |
| 4-5   | E        | In-plane H and P with out-plane C | I+R | 238             |
| 6     | A.1      | Out-plane H, P, and C | I+R | 323             |
| 7     | A.2      | In-plane C | I+R      | 358             |
| 8-9   | E        | In-plane H, P, and C | I+R      | 365             |
| 10-11 | E        | Out-plane C with in-plane H | I+R | 421             |
| 12    | A.1      | Out-plane H, P, and C | I+R      | 434             |
| 13    | A.1      | Out-plane H and C | I+R      | 644             |
| 14-17 | E        | In-plane H | I+R      | 695             |
| 18-21 | E        | In-plane H, P, and C | I+R      | 925             |
| 22-23 | A.1      | In-plane C | I+R      | 1150            |
| 24-27 | E        | In-plane H and C | I+R      | 1237            |
| 28    | A.2      | In-plane C | I+R      | 1352            |
| 29-30 | A.1      | Out-plane H | I+R      | 2130            |
III. The Tc of pristine HPC₃ and biaxial tensile strained HPC₃ as a function of Coulomb pseudopotential μ⁺.

It is well known that the Coulomb pseudopotential μ⁺ is an empirical parameter which is closely associated with Tc. The calculated Tc of pristine HPC₃ and biaxial tensile strained HPC₃ as a function of μ⁺ is shown in Fig. S3. The value of μ⁺ is considered in the range of 0.05–0.25. As is seen in Fig. S3, the Tc decreases monotonically with the increasing of μ⁺ for both pristine HPC₃ and biaxial tensile strained HPC₃. As μ⁺ increases from 0.05 to 0.25, Tc decreases from 38.8 K, 45.9 K, 52.5 K, 66.8 K to 10.5 K, 14.6 K, 21.2 K, 32.1 K for the pristine, 1%, 2%, and 3% tensile strained cases, respectively. For the commonly used μ⁺ = 0.10, the Tc for the pristine, 1%, 2%, and 3% tensile strained cases are 31.0 K, 37.3 K, 44.4 K, and 57.3 K, respectively, which are listed in Table 1 of the main text.

FIG. S3: The calculated Tc of pristine HPC₃ and 1%, 2%, and 3% biaxial tensile strained HPC₃ as a function of Coulomb pseudopotential μ⁺. The vertical line marks the value of μ⁺ = 0.10 used in the main text.

[1] K. Rajput, and D. R. Roy, Phys. Chem. Chem. Phys. 22, 8625 (2020).