Supplementary Materials

Phonon-mediated superconductivity in two-dimensional hydrogenated phosphorus carbide: HPC_3

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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].

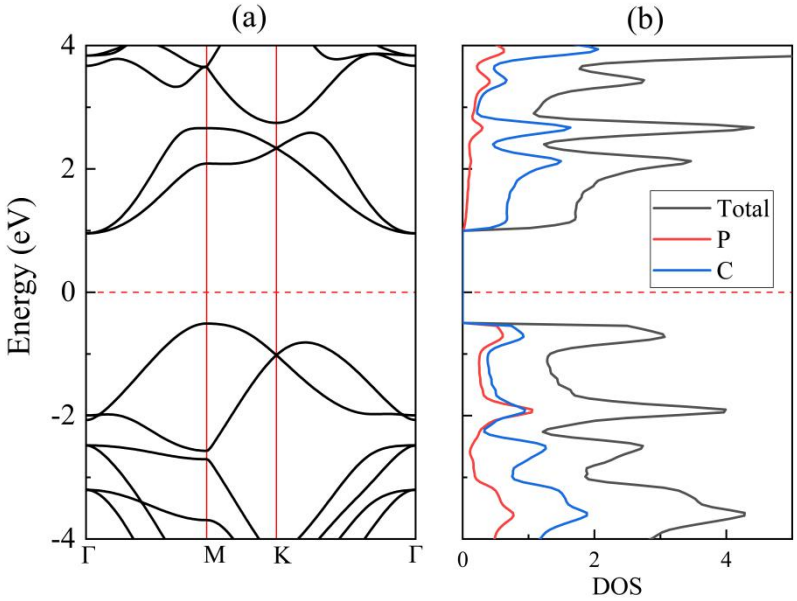

FIG. S1: (a) The electronic band structure of PC_3 along high-symmetry line Γ-M-K-Γ. (b) The total DOS of PC_3 and total DOS of P and C atoms.

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.

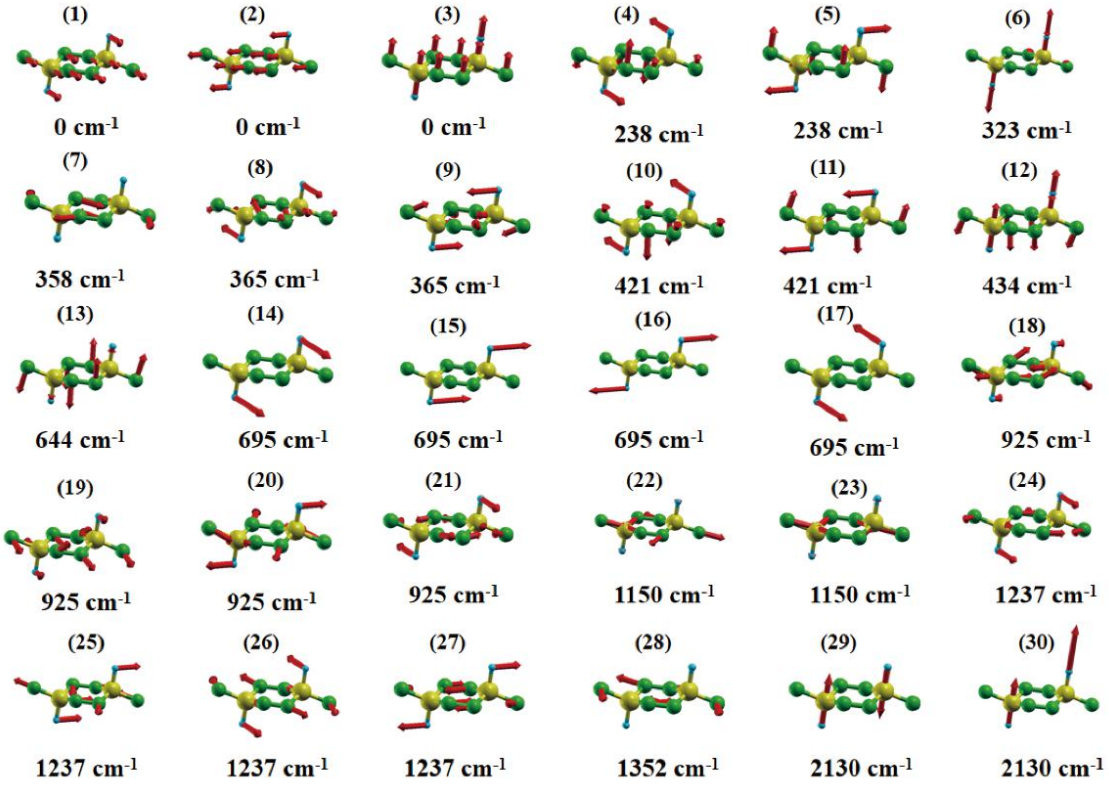

FIG. S2: The thirty vibration modes of pristine HPC_3 at Γ point in the Brillouin zone. The vibration frequencies are shown below each figure. The yellow, green, and blue spheres represent phosphorus, carbon, and hydrogen atoms, respectively, and the red arrow represents the direction of atomic vibration.

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 Γ 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	-	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	-	1352
29-30	A_1	Out-plane H	I+R	2130

III. The Tc of pristine HPC_3 and biaxial tensile strained HPC_3 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 T_c. The calculated T_c of pristine HPC_3 and biaxial tensile strained HPC_3 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 T_c decreases monotonically with the increasing of μ^* for both pristine HPC_3 and biaxial tensile strained HPC3. As μ^* increases from 0.05 to 0.25, T_c 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 $\mu^* = 0.10$, the T_c for the 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.

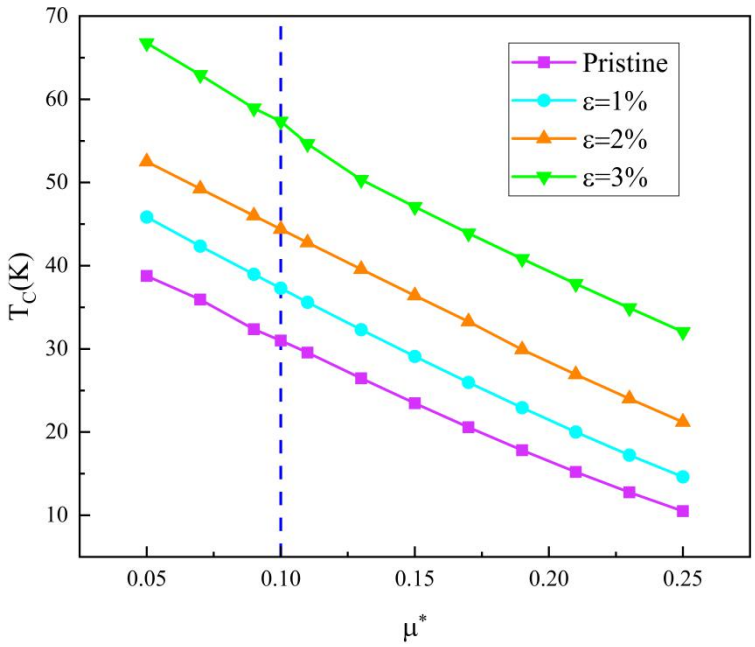

FIG. S3: The calculated T_c of pristine HPC_3 and 1%, 2%, and 3% biaxial tensile strained HPC_3 as a function of Coulomb pseudopotential μ^*. The vertical line marks the value of $\mu^* = 0.10$ used in the main text.

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