Supplementary Information for

Prediction of high-temperature superconductors at ambient pressure with diamond-like structures: B_2CX (X = N, P)

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I. SUPPLEMENTAL FORMULAS

The total EPC constant λ is obtained via isotropic Eliashberg function [1-3]

$$\alpha^2F(\omega) = \frac{1}{2\pi N(E_F)}\sum_{qv} \delta(\omega - \omega_{qv})\frac{\gamma_{qv}}{\omega_{qv}}, \tag{S1}$$

$$\lambda = 2\int \frac{\alpha^2F(\omega)}{\omega}d\omega = \sum_{qv} \lambda_{qv}, \tag{S2}$$

where $\alpha^2\mathrm{F}(\omega)$ is Eliashberg function and $N(E_F)$ is the DOS at the Fermi level, ω_{qv} is the phonon frequency of the vth phonon mode with wave vector $\boldsymbol{q}$, and γ_{qv} is the phonon linewidth [1-3]. The γ_{qv} can be estimated by

$$\gamma_{qv} = \frac{2\pi\omega_{qv}}{\Omega_{\mathrm{BZ}}}\sum_{\boldsymbol{k},n,m} \left|g^{v}_{\boldsymbol{k}n,\boldsymbol{k}+\boldsymbol{q}m}\right|^2 \delta(\varepsilon_{\boldsymbol{k}n} - E_F)\delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}m} - E_F), \tag{S3}$$

where Ω_{BZ} is the volume of the BZ, $\varepsilon_{\boldsymbol{k}n}$ and $\varepsilon_{\boldsymbol{k}+\boldsymbol{q}m}$ indicate the Kohn-Sham energy, and $g^{v}_{\boldsymbol{k}n,\boldsymbol{k}+\boldsymbol{q}m}$ represents the screened electron-phonon matrix element. λ_{qv} is the EPC constant for phonon mode $\boldsymbol{q}v$, which is defined as

$$\lambda_{qv} = \frac{\gamma_{qv}}{\pi\hbar N(E_F)\omega^2_{\boldsymbol{q}v}}. \tag{S4}$$

T_c is estimated by McMillan-Allen-Dynes formula [3]

$$T_c = \frac{\omega_{log}}{1.2}exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]. \tag{S5}$$

The Coulomb repulsion μ^* in Eq.(S5) is set to 0.10 and the logarithmic average of the phonon frequencies ω_{log} is defined as

$$\omega_{log} = exp\left[\frac{2}{\lambda}\int \alpha^2F(\omega)\frac{ln\ \omega}{\omega}d\omega\right]. \tag{S6}$$

Furthermore, to estimate the thermodynamic properties such as critical magnetic field $H_c(0)$, superconducting gap $\Delta(0)$, specific heat jump $\Delta\mathrm{C}(T_c)$ and isotope coefficient β, we used the following semiempirical formulas [4]

$$\frac{\gamma T_c^2}{H_c^2(0)} = 0.168\left[1 - 12.2\left(\frac{T_c}{\omega_{log}}\right)^2 \ln\left(\frac{\omega_{log}}{3T_c}\right)\right], \tag{S7}$$

$$\frac{2\Delta(0)}{k_BT_c} = 3.53\left[1 + 12.5\left(\frac{T_c}{\omega_{log}}\right)^2 \ln\left(\frac{\omega_{log}}{2T_c}\right)\right], \tag{S8}$$

$$\frac{\Delta\mathrm{C}(T_c)}{\gamma T_c} = 1.43\left[1 + 53\left(\frac{T_c}{\omega_{log}}\right)^2 \ln\left(\frac{\omega_{log}}{3T_c}\right)\right], \tag{S9}$$

$$\beta = \frac{1}{2}\left[1 - \frac{1.04(1+\lambda)(1+0.62\lambda)}{[\lambda - \mu^*(1+0.62\lambda)]^2}\mu^{*2}\right], \tag{S10}$$

here k_B is the Boltzmann constant and γ is the Sommerfeld constant, which can be obtained by

$$\gamma = \frac{2}{3}\pi^2k_B^2N(E_F)(1+\lambda). \tag{S11}$$

II. SUPPLEMENTAL FIGURES

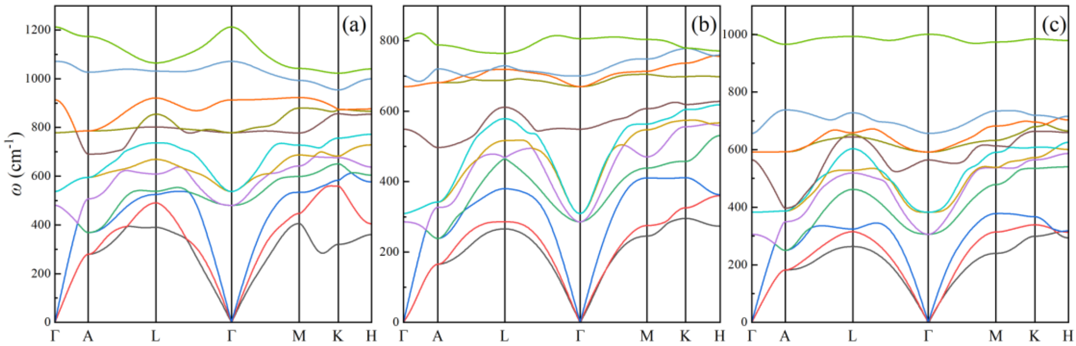

Fig. S1. Phonon spectra of (a) d-B_2CN, (b) d-B_2CP-I and (c) d-B_2CP-II.

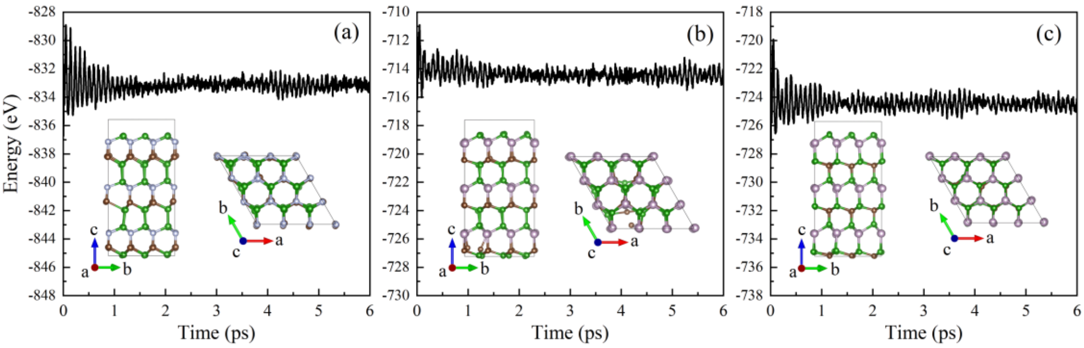

Fig. S2. AIMD simulations of (a) d-B_2CN, (b) d-B_2CP-I and (c) d-B_2CP-II at 300 K.

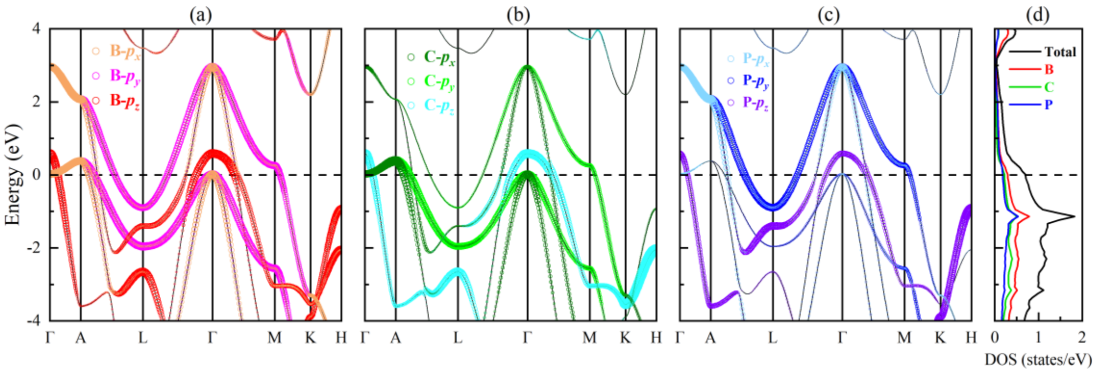

Fig. S3. Orbital-projected band structures of (a) B, (b) C and (c) P for d-B_2CP-II along the high-symmetry line Γ-A-L-Γ-M-K-H. (d) Total DOS of d-B_2CP-II, B, C and P.

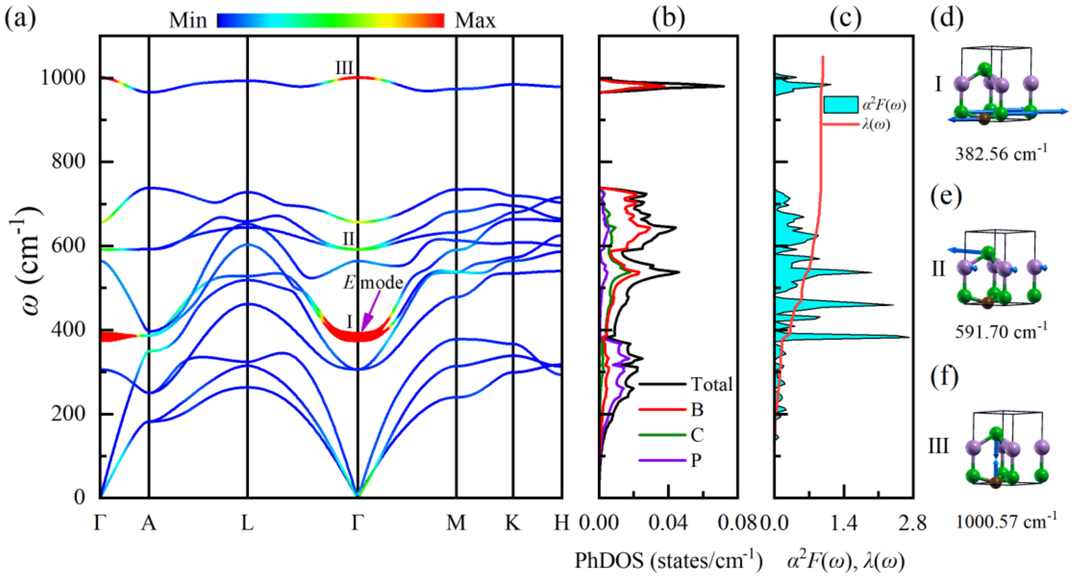

Fig. S4. (a) Phonon dispersion weighted by the magnitude of EPC λ_{qv}, (b) PhDOS, (c) Eliashberg spectral function $\alpha^2F(\omega)$ and cumulative frequency dependence of EPC $\lambda(\omega)$ for d-B_2CP-II. (d)-(f) Its VMs for the prominent λ_{qv} I, II and III, respectively.

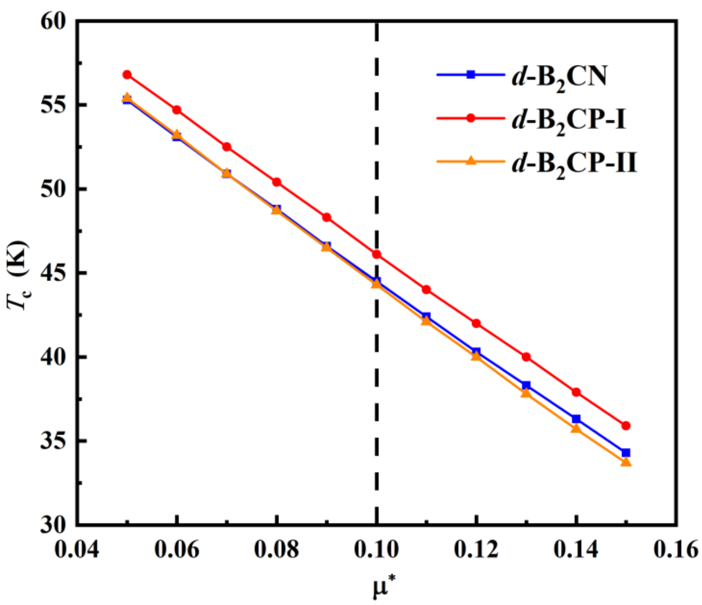

Fig. S5. Critical temperature T_c as a function of Coulomb pseudopotential μ^* for d-B_2CN, d-B_2CP-I and d-B_2CP-II. The vertical line marks the value μ^* = 0.10 used in this work.

Notes and references

1 W. McMillan, *Phys. Rev. B*, 1968, **167**, 331.

2 R. Dynes, *Solid State Commun.*, 1972, **10**, 615.

3 P. B. Allen and R. Dynes, *Phys. Rev. B*, 1975, **12**, 905.

4 J. Carbotte, *Rev. Mod. Phys.*, 1990, **62**, 1027.