Supporting Information for: Insight into Two-Dimensional Borophene: Five-Center Bond and Phonon-Mediated Superconductivity

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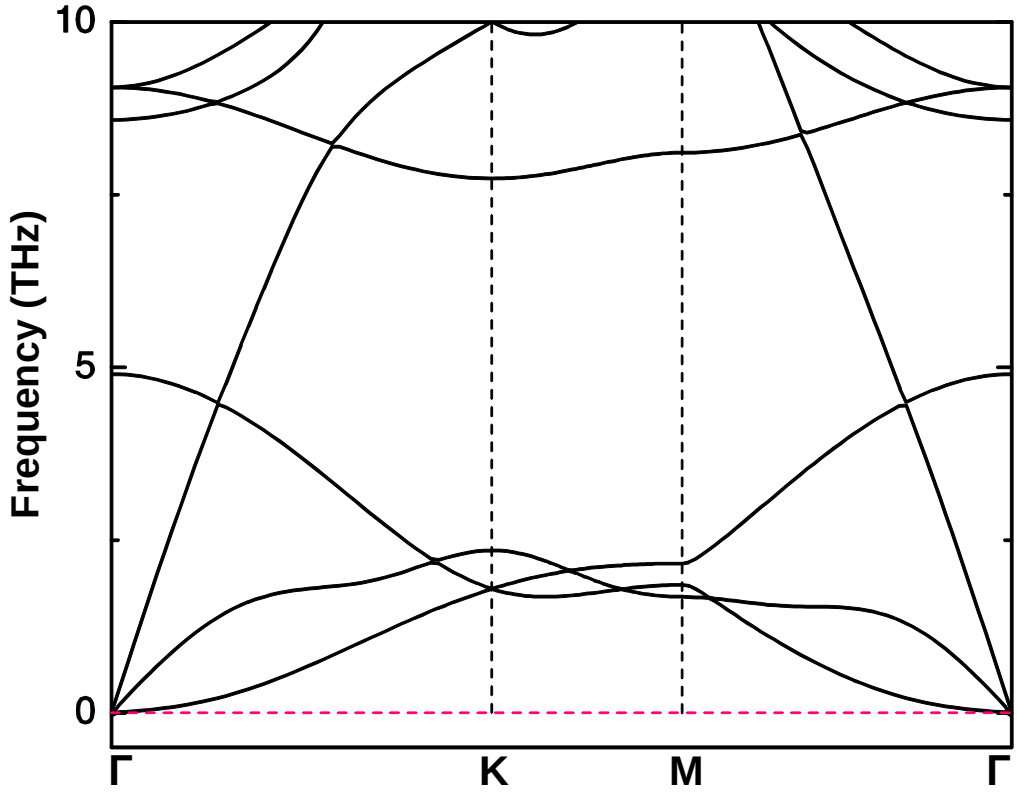

Figure S1: Amplification of phonon dispersion of super-B below 10 THz. Around the Γ point, there are two linear LA and TA acoustic phonon branches, and a parabolic ZA mode. All frequencies are free from imaginary, confirming the dynamical stability of super-B.

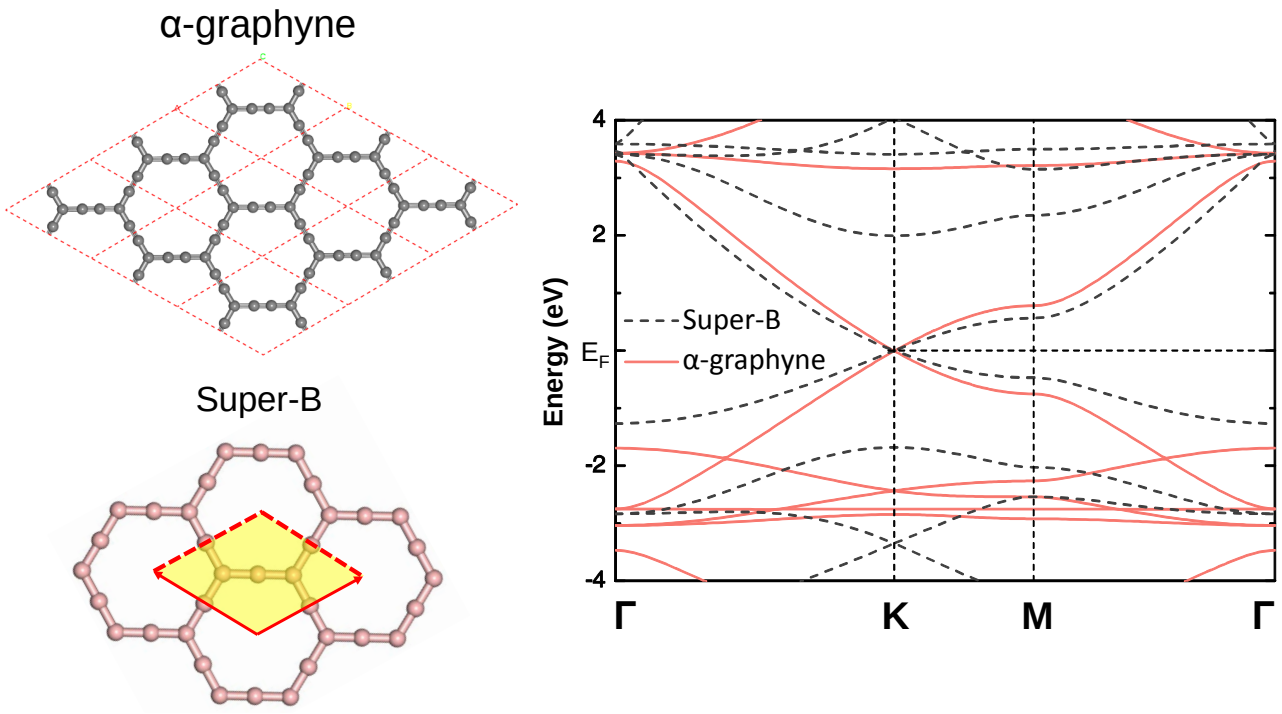

Figure S2: Crystal structure of α-graphyne and super-B. Electronic band structures of pristine α-graphyne and super-B under -0.2 e/B doping. Both are Dirac materials.

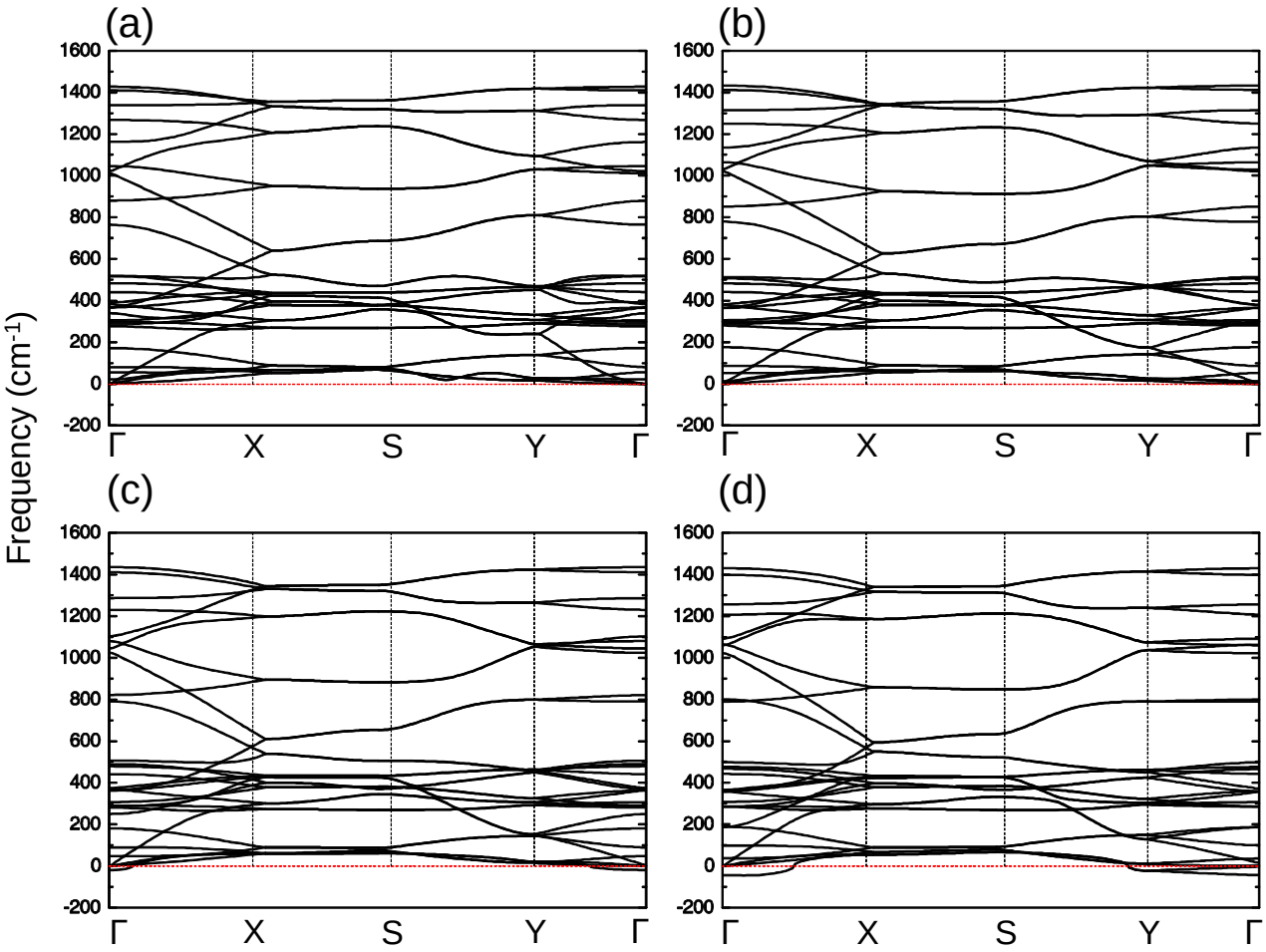

Figure S3: Phonon dispersions of super-B under uniaxial strain of (a) ε=6%, (b) ε=8%, (c) ε=10%, (d) ε=12%.

Table S1: Calculated properties of singled-walled borophene nanotubes (SWBNTs). N_{atom} is the number of atoms. E_g is the electronic band gap. E_c is the cohesive energy and D is the diameter of SWBNTs.

SWBNTs	N_{atom}	E_g (eV)	E_c (eV/atom)	D (Å)
(4,0)	40	0, metal	5.256	7.07
(8,0)	40	0, metal	5.537	13.91
(4,4)	80	0, metal	5.284	11.93
(8,8)	80	0, metal	5.543	23.99

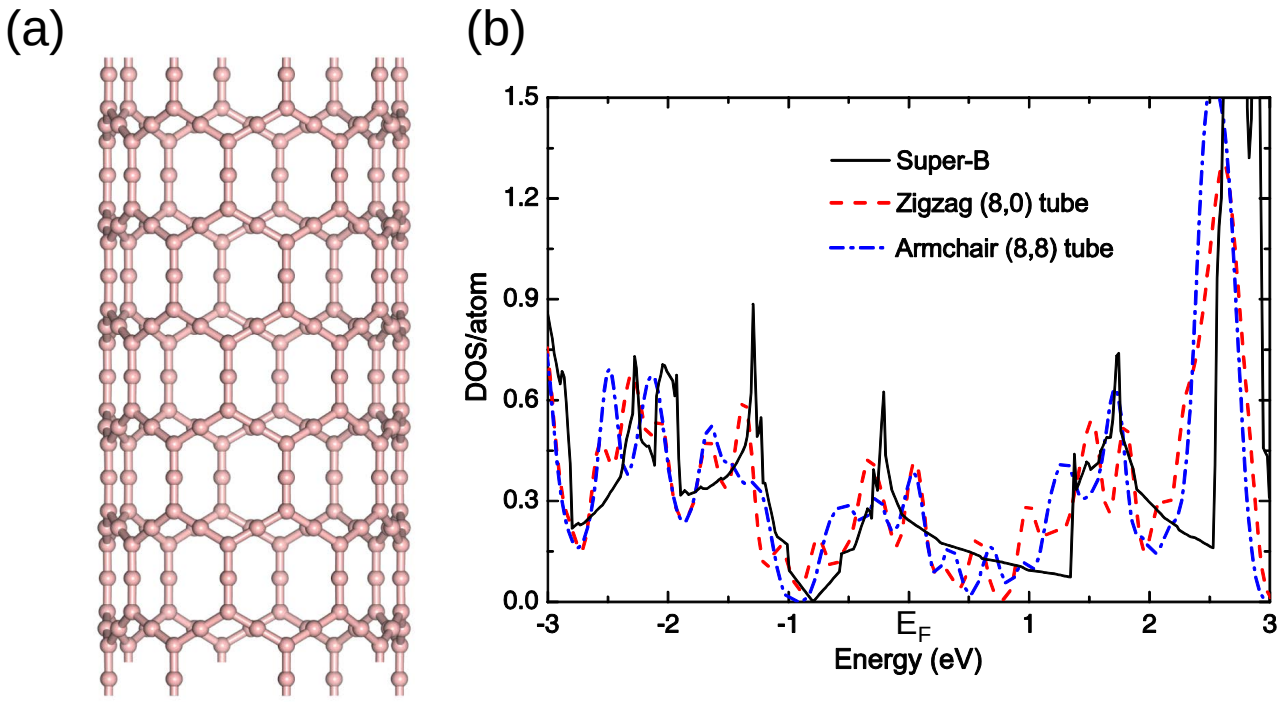

Figure S4: (a) Optimized super-borophene nanotubes of zigzag (8,0) as an example. All singled-walled borophene nanotubes (SWBNTs) are cylindrical without any buckling or collapse in our study. (b) Electronic density of states of planar super-borophene, zigzag (8,0) and armchair (8,8) nanotubes, indicating the metallic property of SWBNTs.

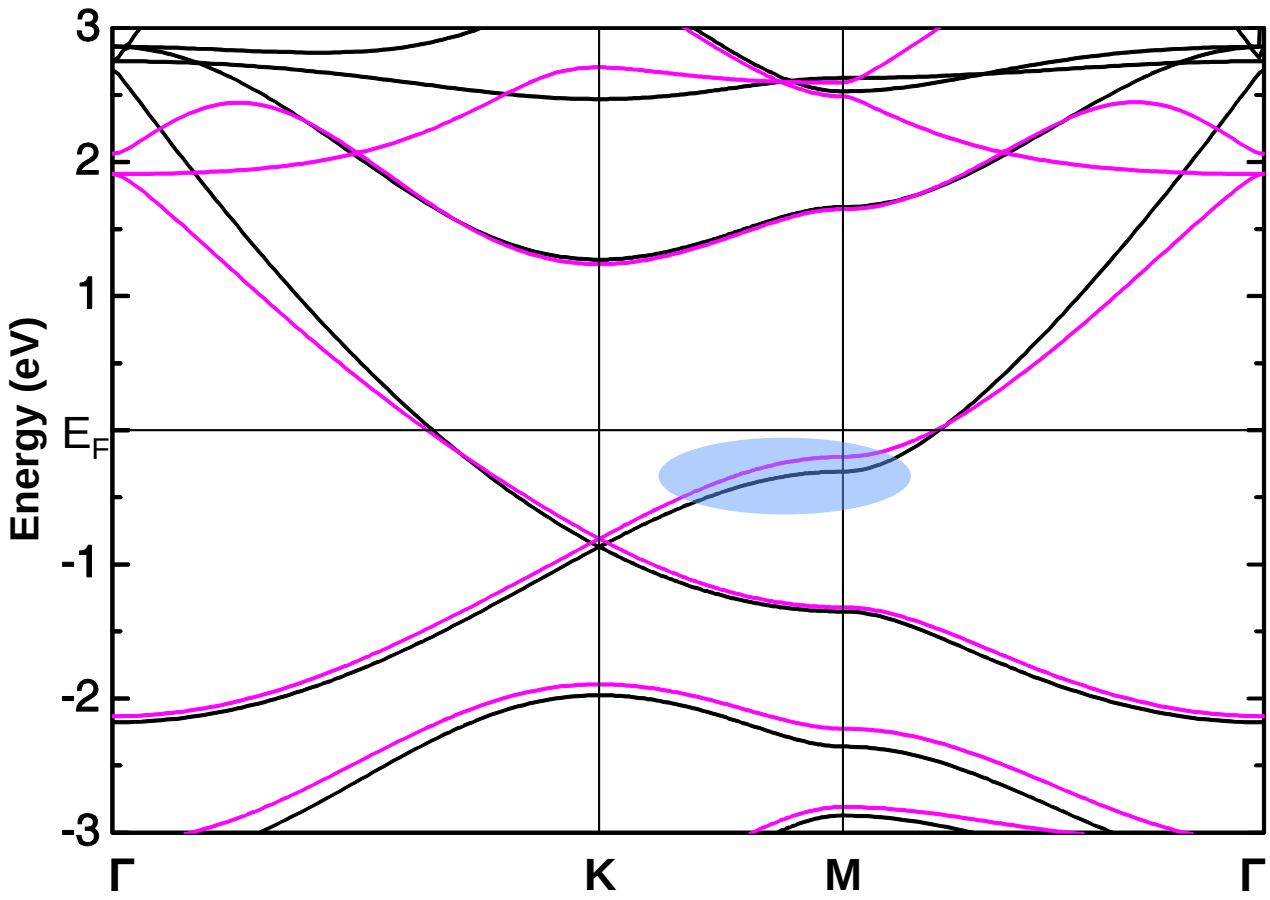

Figure S5: Band structure of the undistorted (black lines) and distorted structures (pink lines) in super-B by the O_z phonon mode ($u_B \approx 0.4$ Å) in super-B.