Supporting Information:

Multiple Dirac Cones in BN Co-doped *β*-graphyne

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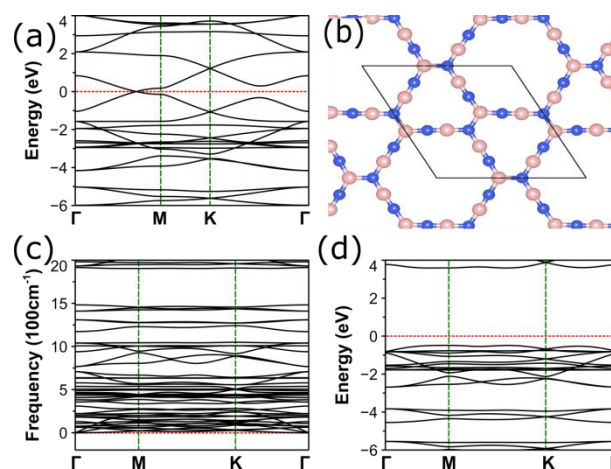

Fig. S1. (a) The band structure of *β*-graphyne. (b) The geometry structure, (c) phonon spectrum and (d) band structure of BN analogue of *β*-graphyne with P-62m symmetry (named β-GY$_{BN3}$). The pink and blue balls stand for B and N atoms, respectively.
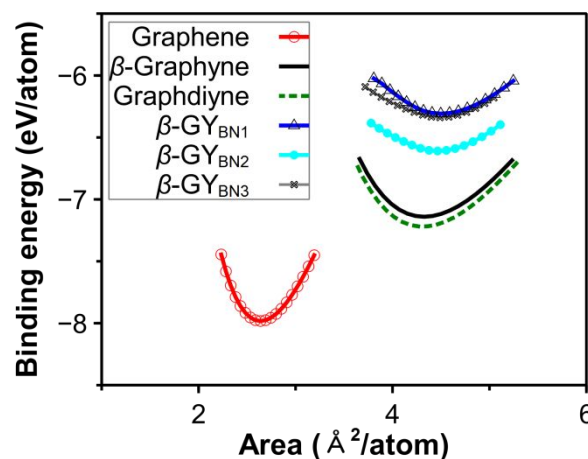

Fig. S2. The binding energy per atom as a function of 2D crystal area per atom for graphene, *β*-graphyne (*β*-GY), graphdiyne, β-GY$_{BN1}$, β-GY$_{BN2}$ and β-GY$_{BN3}$.
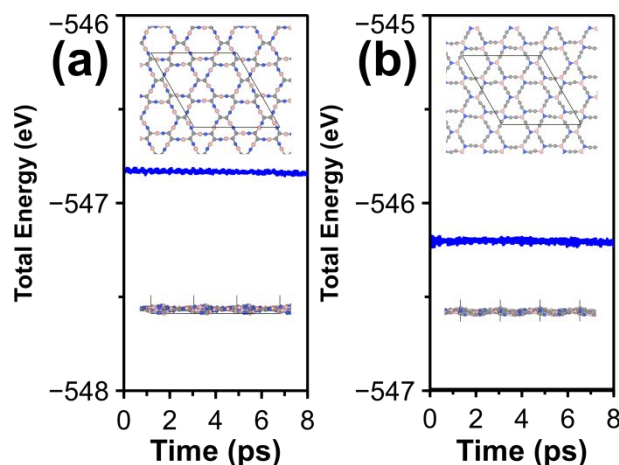
Fig. S3. *Ab initio* molecular dynamics (AIMD) simulations of 2×2 (a) β-GY$_{BN1}$ and (b) β-GYBN2 for 8 ps after equilibration with a time step of 0.75 fs at 1000 K. The insets are the top-view and side-view snapshots of their atomic configurations at the end of AIMD simulations.
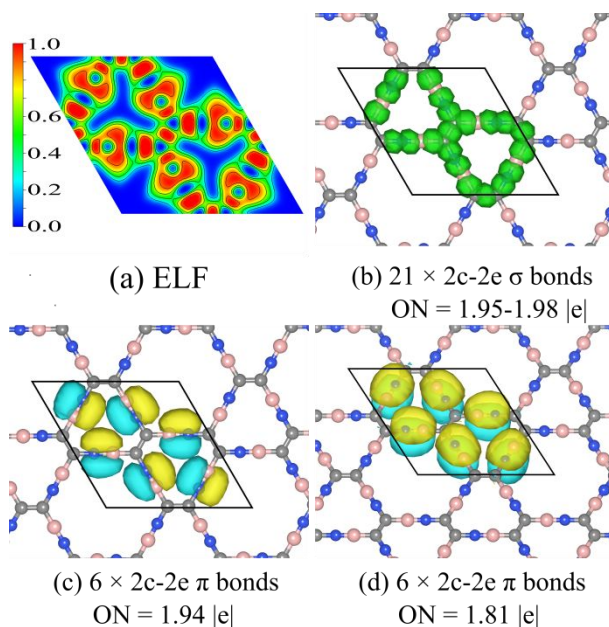

(a) ELF

(b) 21 × 2c-2e σ bonds
ON = 1.95-1.98 |e|

(c) 6 × 2c-2e π bonds
ON = 1.94 |e|

(d) 6 × 2c-2e π bonds
ON = 1.81 |e|

Fig. S4. (a) Electron localization function (ELF) maps sliced in the atomic plane of β-GY$_{BN1}$. (b-d) Two center two-electron (2c-2e) bonding patterns of β-GY$_{BN1}$ by solid state adaptive natural density partitioning (SSAdNDP) method. In the ELF maps, the colors of red and blue refer to the highest (1.0) and lowest value (0.0) of ELF, and ON is the abbreviation of occupation number.
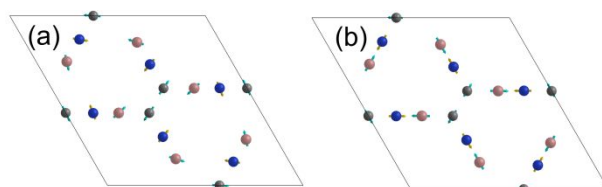

Fig. S5. Atomic displacements of the Raman-active phonons with frequency of (a) 1232 cm^{-1} and (b) 1897 cm^{-1} for β-GY$_{BN1}$.