

Ambient-pressure superconductivity above 22 K in hole-doped YB₂

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I. The Sum of projected DOS for Selected Atoms and orbitals in YB₂

The orbital compositions of elements B and Y in YB₂, along with their projected DOS, are displayed in Fig. S1(a) and (b). In YB₂, the B-*pz*, Y-*dxy* and Y-*dx²* orbitals dominate the total DOS at the Fermi energy level, with the remaining orbitals comprising a minor fraction.

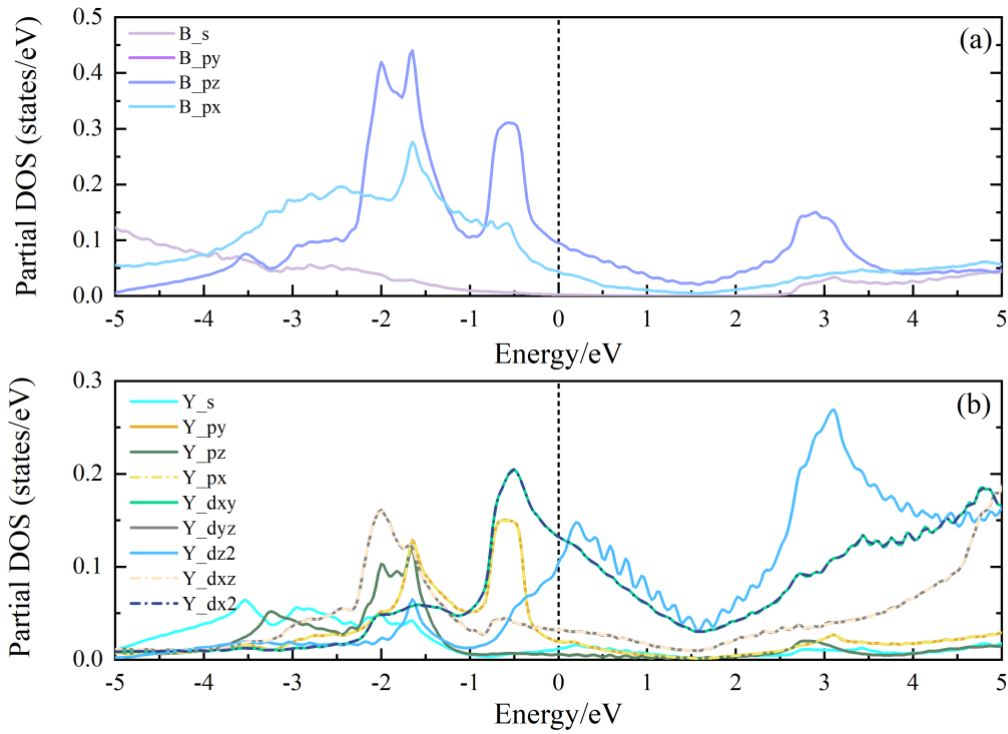


FIG.S1. The projected DOS consisting of individual orbitals of the elements in YB₂. (a) The projected DOS consisting of individual orbitals of the element B in YB₂ is near the E_F , where the dark purple, purple-blue, and blue lines stand in for the B-*py*, B-*pz*, and B-*px* orbitals, respectively, and the purple-grey line represents the s-orbital of element B. (b) In YB₂, the projected DOS of individual element Y orbitals is close to the E_F , where the lines colored bright blue, orange, dark green, and yellow represent the Y-*s*, Y-*py*, Y-*pz*, and Y-*px* orbits; and the other lines colored light green, gray, light blue, light flesh, and dark blue represent the Y-*dxy*, Y-*dyz*, Y-*dz²*, Y-*dxz*, and Y-*dx²* orbits, respectively.

II. The Eliashberg spectral function in YB₂ with various additional electron or hole concentrations

The Eliashberg spectral function $\alpha^2F(\omega)$ of YB_2 with different concentrations of electrons and holes added are shown on Fig.S2, Fig. S3 and Fig. S4, respectively. When insertion electron concentration increases, the peak values of mid-frequency phonon and occupied areas of the Eliashberg spectral function increase slightly, but the high-frequency optical phonon and the peak values of low-frequency acoustic phonon and occupied areas decrease significantly. Furthermore, the peaks and occupied areas of the mid-frequency phonon bands decrease slightly as the concentration of additional holes in YB_2 rises, while the peaks and occupied areas of the Eliashberg spectral functions of the low-frequency acoustic and high-frequency optical phonons increase dramatically, particularly in the acoustic phonon portion. In contrast, the peaks and the area occupied by the Eliashberg spectral function of the acoustic phonon band considerably drop with the addition of hole concentration up to 0.8, and the associated T_c declines steeply.

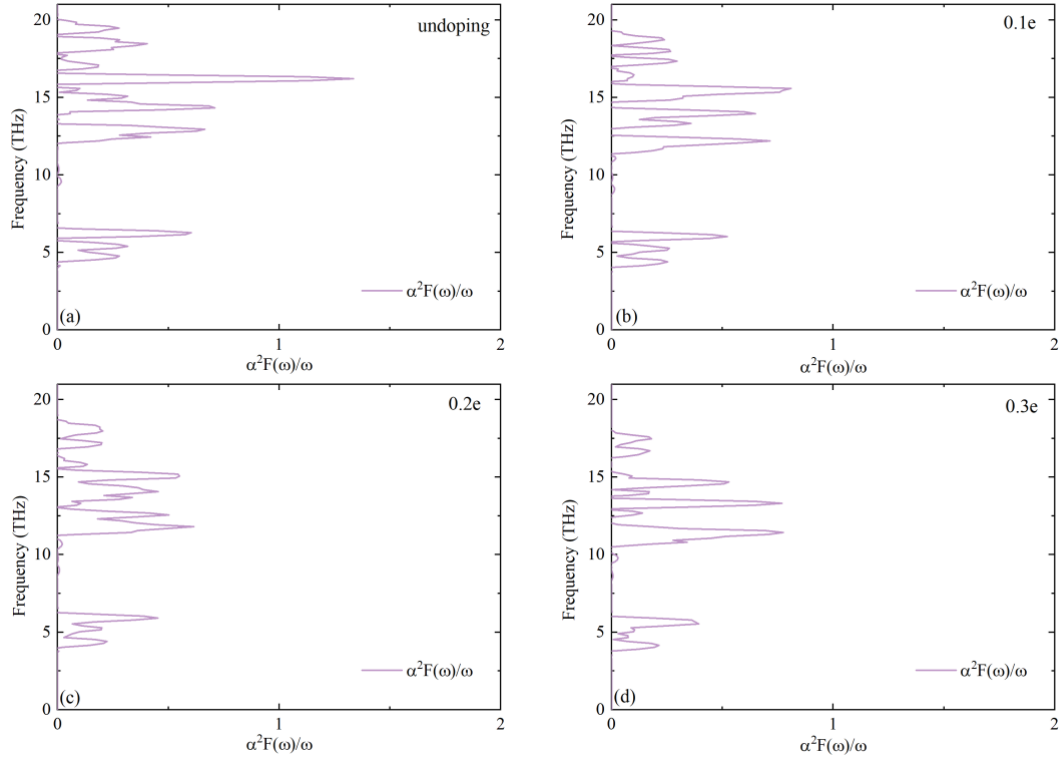


FIG.S2. The Eliashberg spectral function of YB_2 with the addition of different concentrations of electrons(0 ~ 0.3). The Eliashberg spectral function of (a) undoping YB_2 , (b) 0.1 electrons added YB_2 , (c) 0.2 electrons added YB_2 and (d) 0.3 electrons added YB_2 .

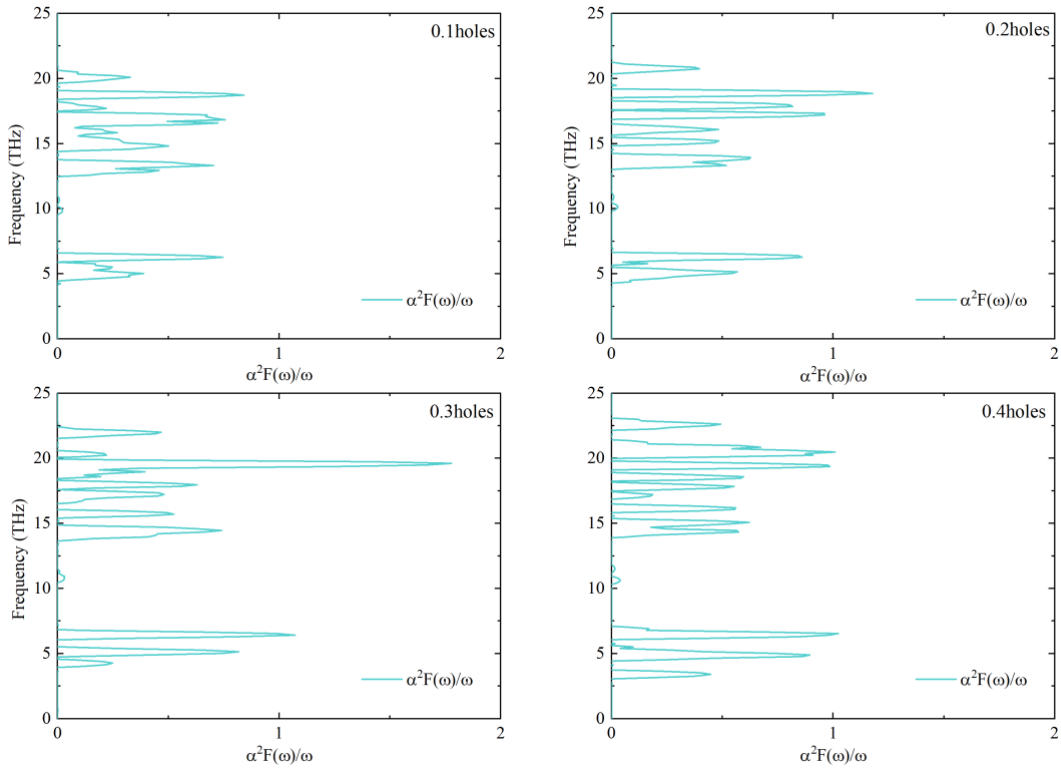


FIG.S3. The Eliashberg spectral function of YB_2 with additional holes at varying concentrations(0.1 ~ 0.4). The Eliashberg spectral function of (a) YB_2 with 0.1 holes added, (b) YB_2 with 0.2 holes

added, (c) YB₂ with 0.3 electrons added and (d) YB₂ with 0.4 electrons added.

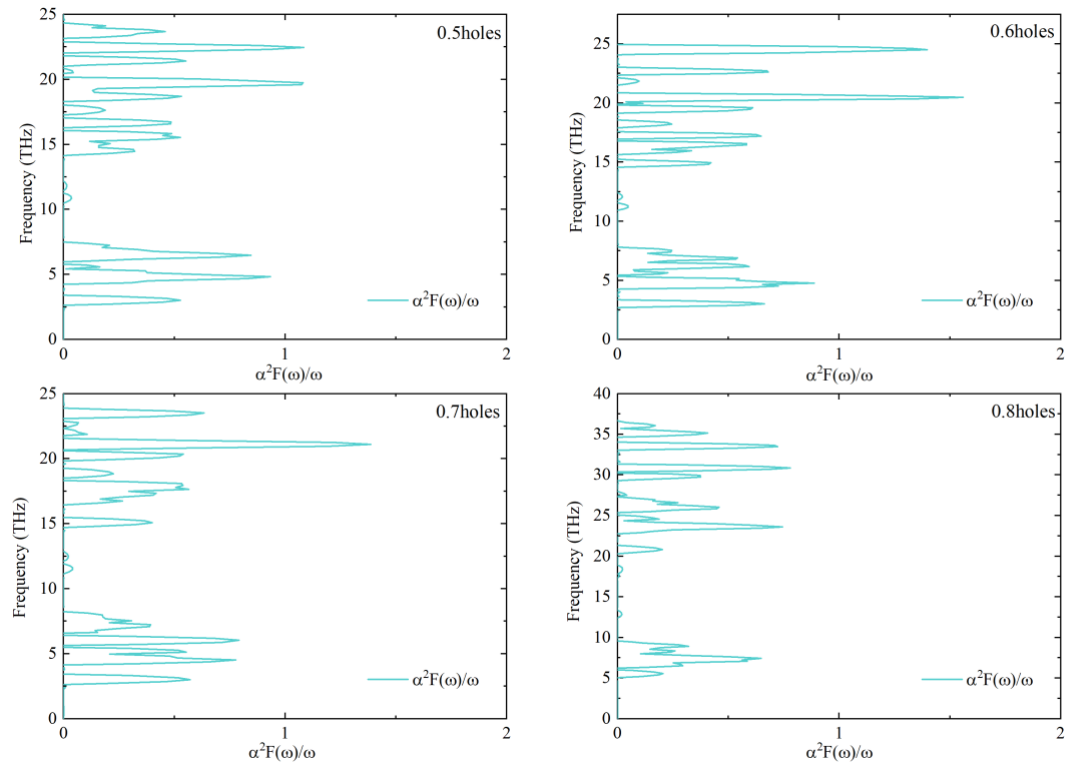


FIG.S4. The Eliashberg spectral function of YB₂ with additional holes at varying concentrations(0.5 ~0.8). The Eliashberg spectral function of (a) YB₂ adding 0.5 holes, (b) YB₂ adding 0.6 holes, (c) YB₂ adding 0.7 holes and (d) YB₂ adding 0.8 holes.