Supplementary information

Pressure-induced flat-bands in one-dimensional moiré superlattices of collapsed chiral carbon nanotubes

Xianliang Zhou[1,2*], Yi Chen[1,2], Jiajun Chen[1,2], Cheng Hu[1,2], Bosai Lyu[1,2], Kunqi Xu[1,2], Shuo Lou[1,2], Peiyue Shen[1,2], Saiqun Ma[1,2], Zhenghan Wu[1,2], Yufeng Xie[1,2], Zhichun Zhang[1,2], Zhiguo Lü[1,2], Weidong Luo[1,2,3], Qi Liang[1,2,4], Lede Xian[5,6*], Guangyu Zhang[5,7,8], Zhiwen Shi[1,2,4*]

[1]Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Shenyang National Laboratory for Materials Science, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

[2]Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China

[3]Institute of Natural Sciences, Shanghai Jiao Tong University, Shanghai 200240, China

[4]Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, 200240, China

[5]Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China

[6]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany

[7]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

[8]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

[*]fishballien@sjtu.edu.cn (X.Z.); xianlede@sslab.org.cn (L.X.); zwshi@sjtu.edu.cn (Z.S.)

1. Pressure-induced flat-bands in the collapsed metallic (62, 2) CNT

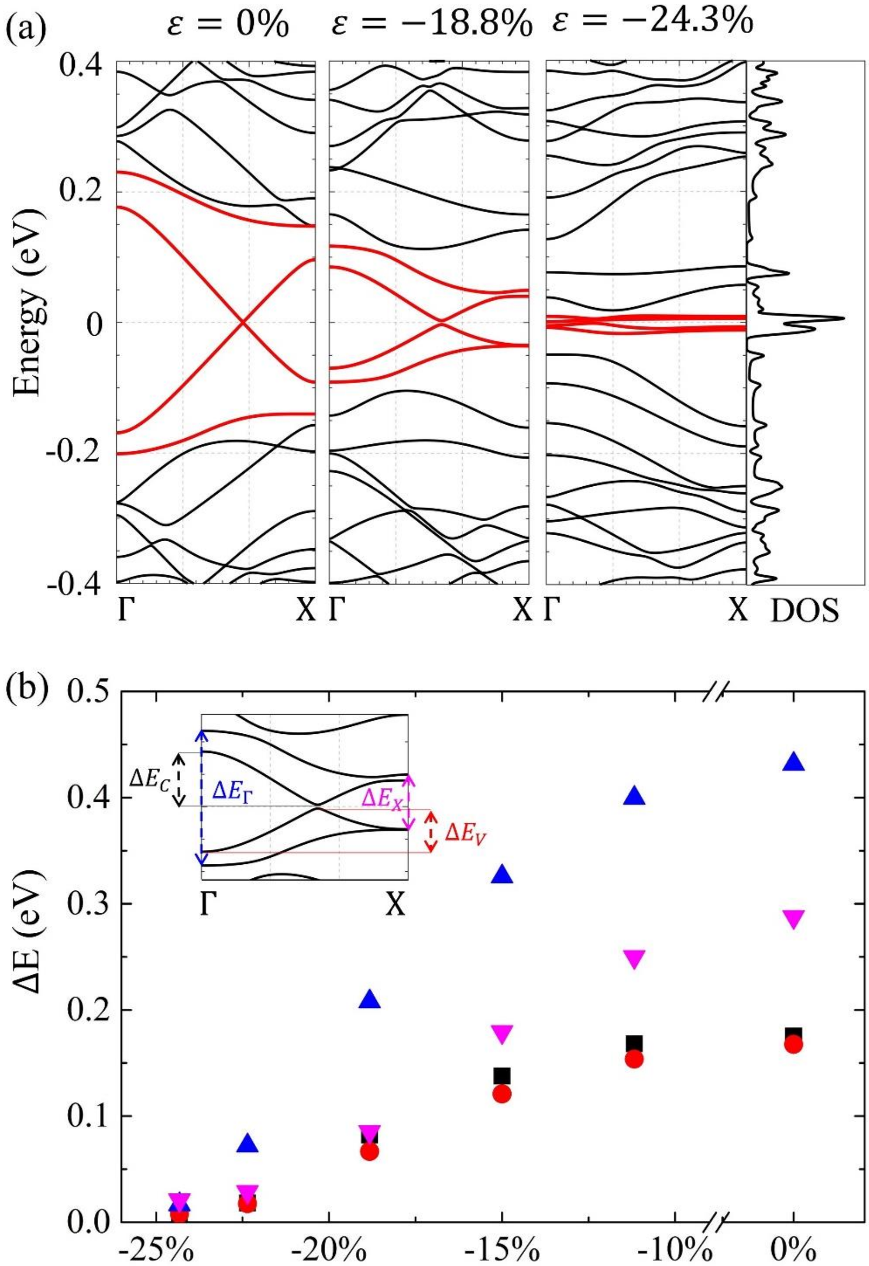

Figure. S1. (a) Evolution of band structure of the collapsed metallic (62, 2) CNT under external compression with four central bands highlighted in red. The density of states at $\varepsilon = -24.3\%$ is shown on the right panel in (a). (b) Energy span and bandwidth of the collapsed metallic (62, 2) CNT as a function of the compression strain. The energy span of the central four bands at Γ and X, ΔE_{Γ} and ΔE_X, and the bandwidth of the lowest conduction band and the highest valence band, ΔE_C and ΔE_V. Inset schematically represents these four quantities. Notably, at a critical compression of $\varepsilon = -24.3\%$, all the four quantities drop to near zero.

2. Explicit expression of the critical pressure as a function of chiral angles

Through the Eq. (6) in the main text, an explicit expression for the critical compression $\varepsilon_c(\theta)$ on the chiral angle θ of the CNTs can be derived as

$$\varepsilon_c(\theta) = \sqrt{\frac{\gamma_1^2}{4\gamma_2^2} + \frac{\gamma_0}{\gamma_2} \times \left(\frac{2\theta}{\theta_0} - 1\right)} - \frac{\gamma_1}{2\gamma_2}, \tag{S1}$$

where γ_n are quadratic fitting parameters of the interlayer hopping, and θ_0 is the moiré twisted angle at zero pressure.

Combining the Eq. (5) in the main text and the Eq. (S1), the critical pressure $P_c(\theta)$ dependence on the chiral angles θ of the CNTs can be derived as

$$P_c(\theta) = A\left[e^{-B\times\left(\sqrt{\frac{\gamma_1^2}{4\gamma_2^2} + \frac{\gamma_0}{\gamma_2} \times \left(\frac{2\theta}{\theta_0} - 1\right)} - \frac{\gamma_1}{2\gamma_2}\right)} - 1\right], \tag{S2}$$

where A and B are the exponential fitting parameters mentioned in the main text.

Note that the chiral angle θ is related to the chiral index (n, m) in the CNTs through

$$\theta = \arccos\left(\frac{2n+m}{2\sqrt{n^2+nm+m^2}}\right). \tag{S3}$$

Combining the Eq. (S1), Eq. (S2) and Eq. (S3), we can plot the critical compression, critical pressure dependence on the chiral index for various collapsed chiral CNTs as shown in Figure 5b in the main text.