Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Strong mechanical anisotropy and an anisotropic Dirac state in two-dimensional C_5N_3

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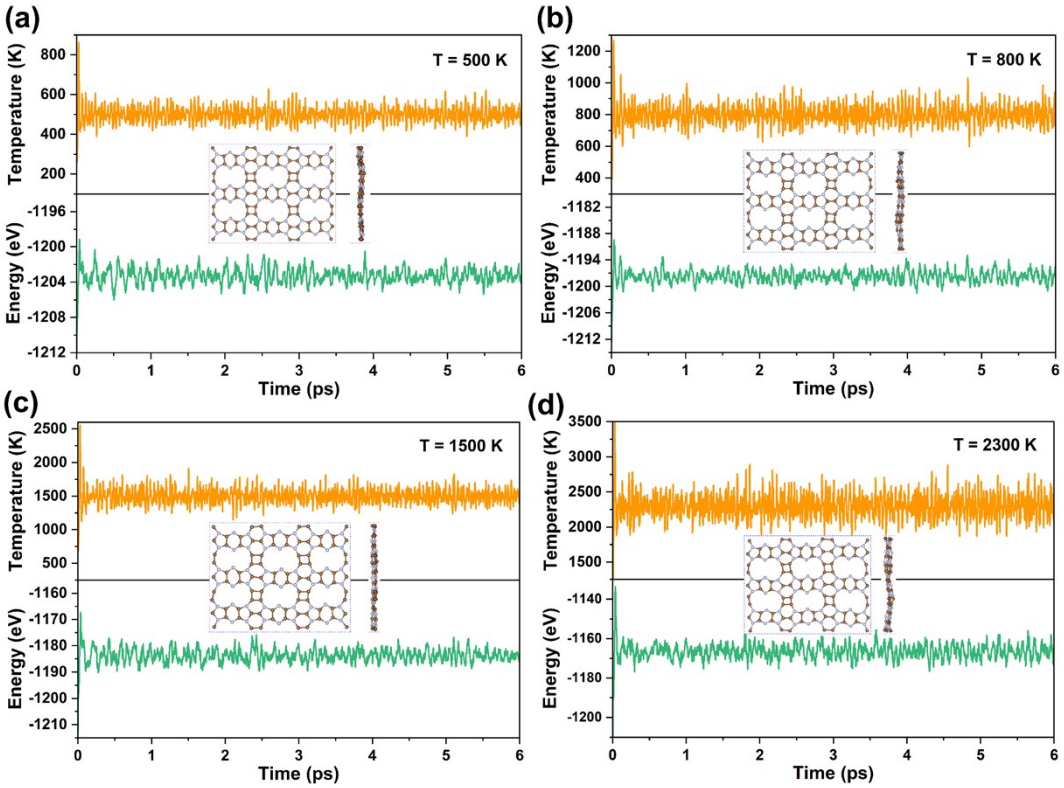

Fig. S1: Temperature and total energy fluctuations of the TPH-C_5N_3 monolayer throughout the AIMD simulation at temperatures of (a) 500 K, (b) 800 K, (c) 1000 K, and (d) 2300 K. Insets display the atomic configurations of TPH-C_5N_3 at these respective temperatures (500, 800, 1500, and 2300 K).

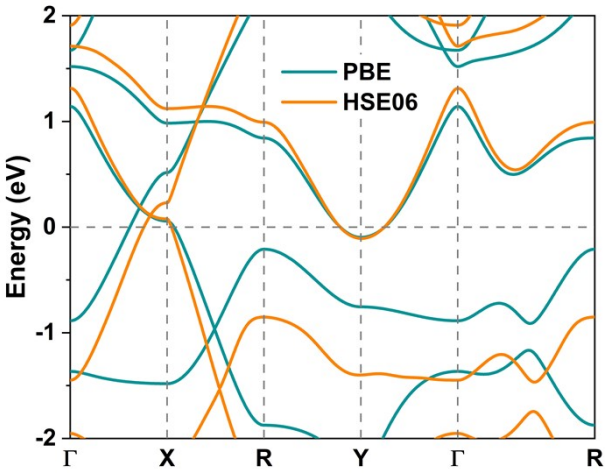

Fig. S2: Band structures of TPH-C_5N_3 monolayer calculated using the PBE (green lines) and HSE06 (yellow lines) functionals.

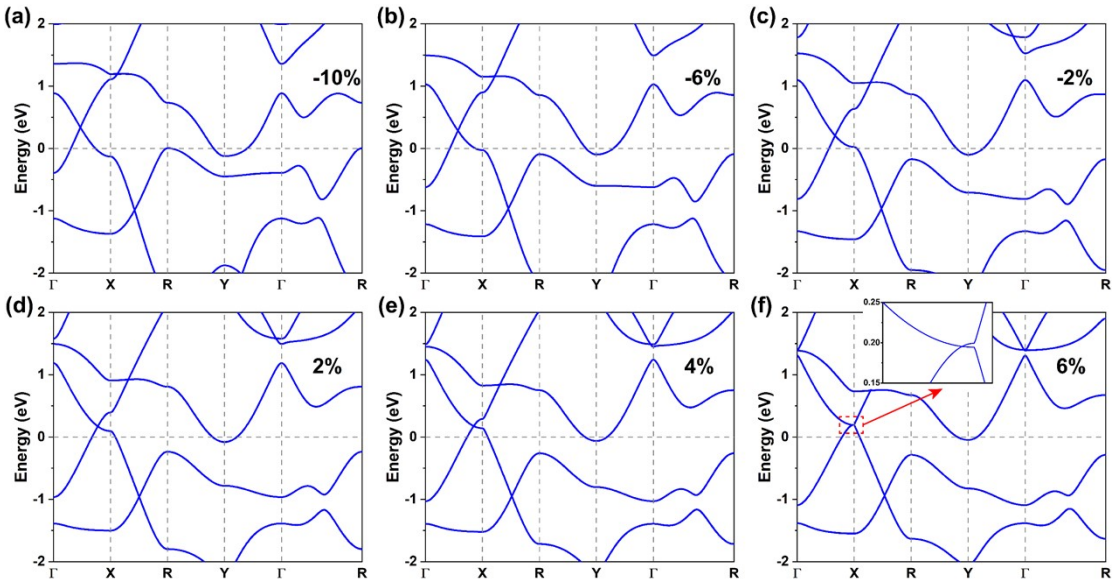

Fig. S3: The effect of uniaxial strain along the *a* axis on the Dirac state of TPH-C_5N_3 in the PBE functional.

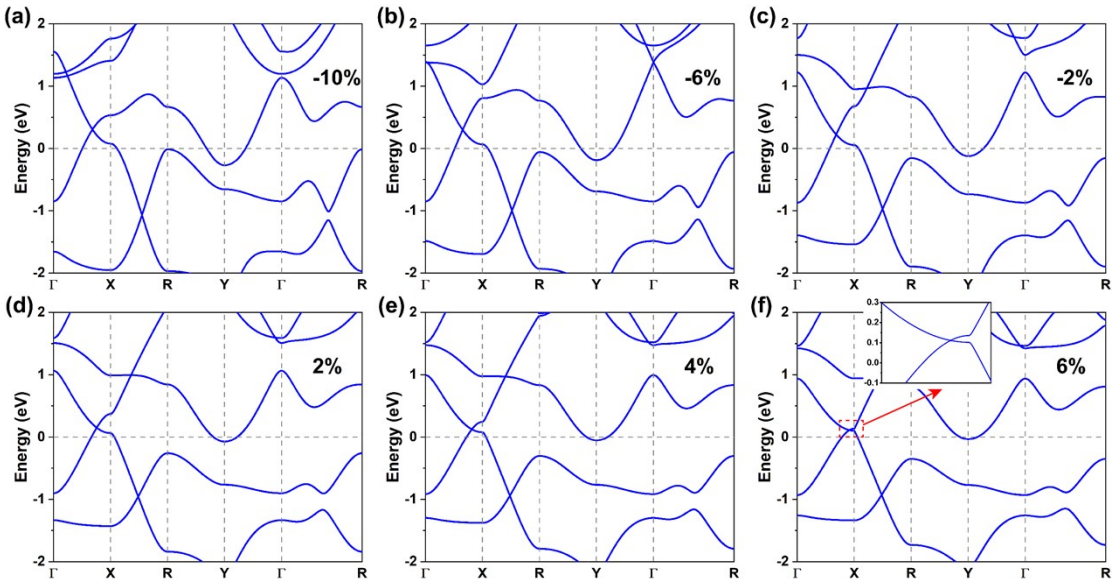

Fig. S4: The effect of biaxial strain on the Dirac state of TPH-C_5N_3 in the PBE functional.