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


# Structural, Elastic and Electronic Properties of Atomically Thin Pyridyne: Theoretical Predictions

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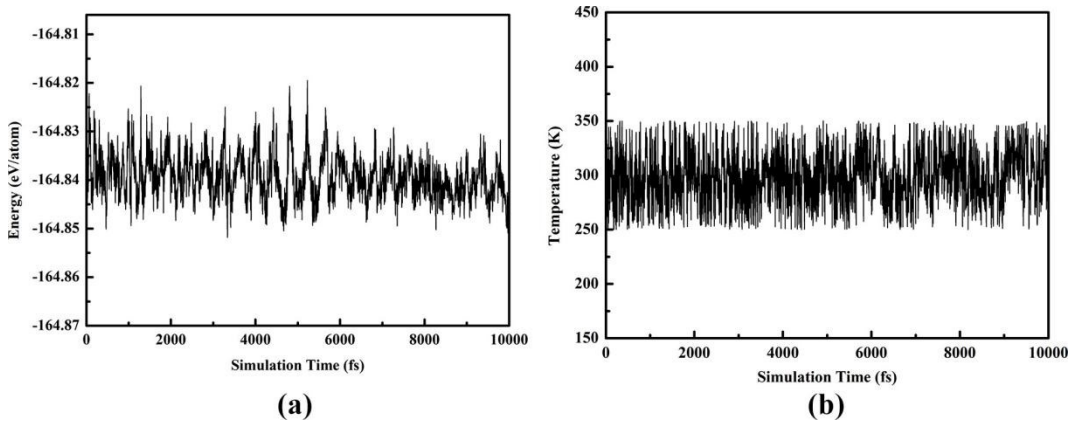


**Fig. S1.** (a) and (b) show total energy and temperature fluctuations of pyridyne at 300 K, respectively.

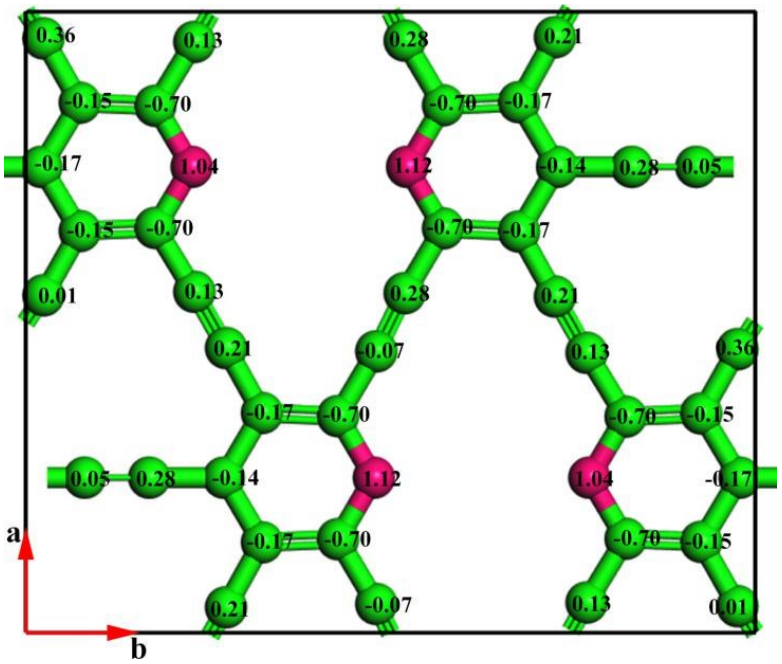


**Fig. S2.** The bader atomic charge of each atom in pyridyne, and the unit is electron charge (*e*).

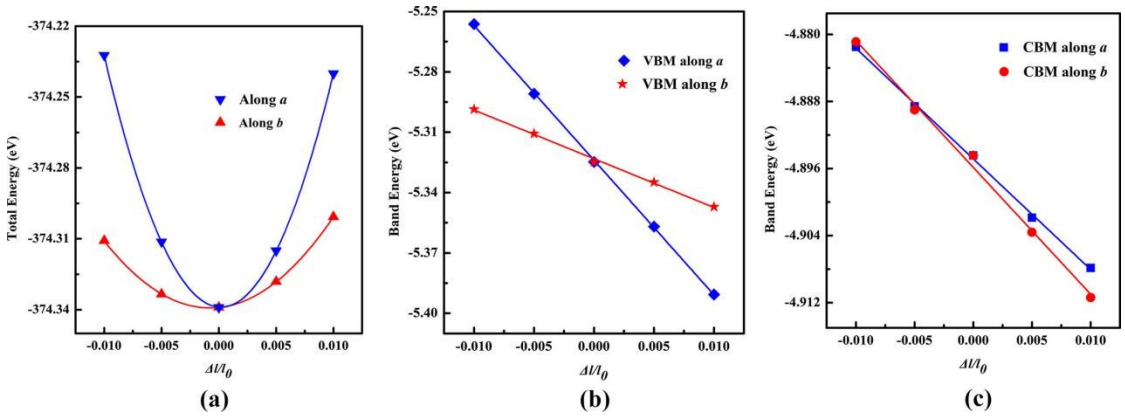


**Fig. S3.** (a) Strain-total energy relations and the energy shifts of (b) VBM and (c) CBM with respect the vacuum energy under uniaxial strain along the *a* and *b* directions for pyridyne.