Eletronic Supplementary information

for

First-principles study of structural, elastic and electronic properties of naphyne and naphdiyne

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Table S1 The energy values of E_{sheet}, $E_{C,\ atom}$, and $\mu_{C,\ atom}$ used for calculating cohesive energy and formation energy.

	E_{sheet}(NY)	E_{sheet}(NDY)	$E_{C,\ atom}$	$\mu_{C,\ atom}$
Energy (eV)	-310.32	-441.36	-1.37	-9.22

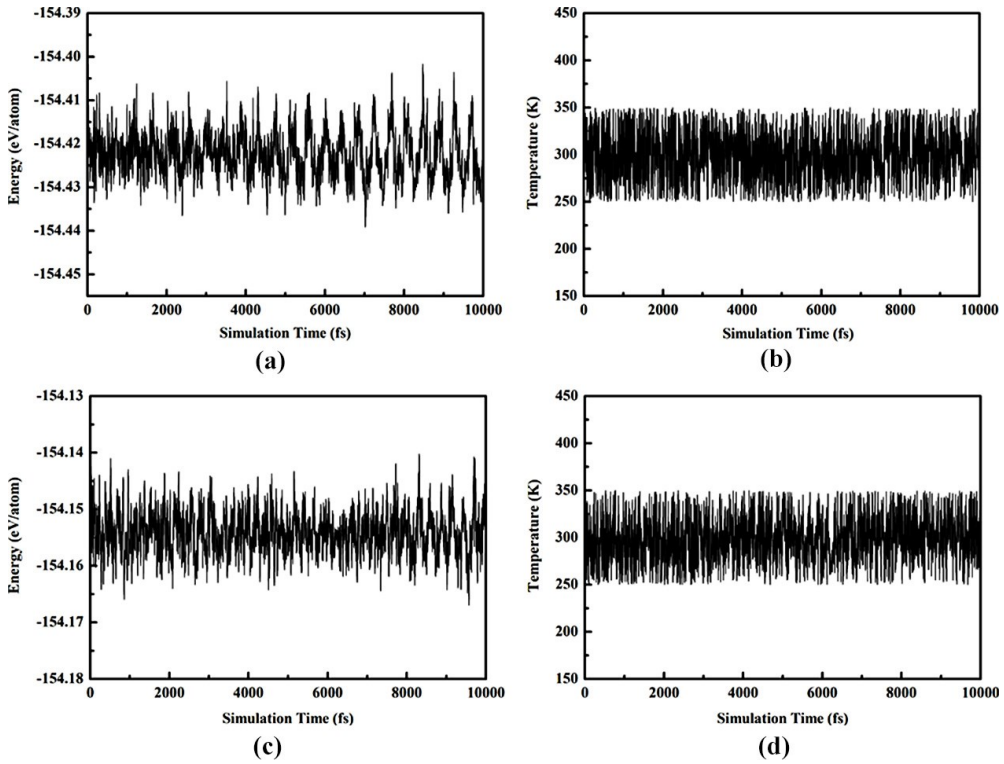

Figure S1. (a), (b), (c), and (d) show total energy and temperature fluctuations of naphyne and naphdiyne at 300 K, respectively.

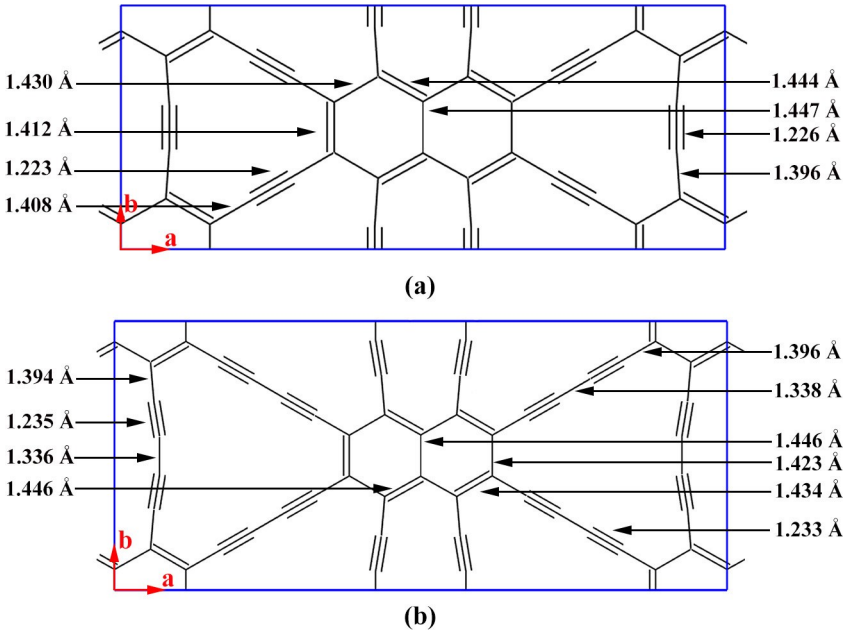

Figure S2. Equilibrium bond lengths of aromatic, single and triple bonds in (a) naphyne and (b) naphdiyne.

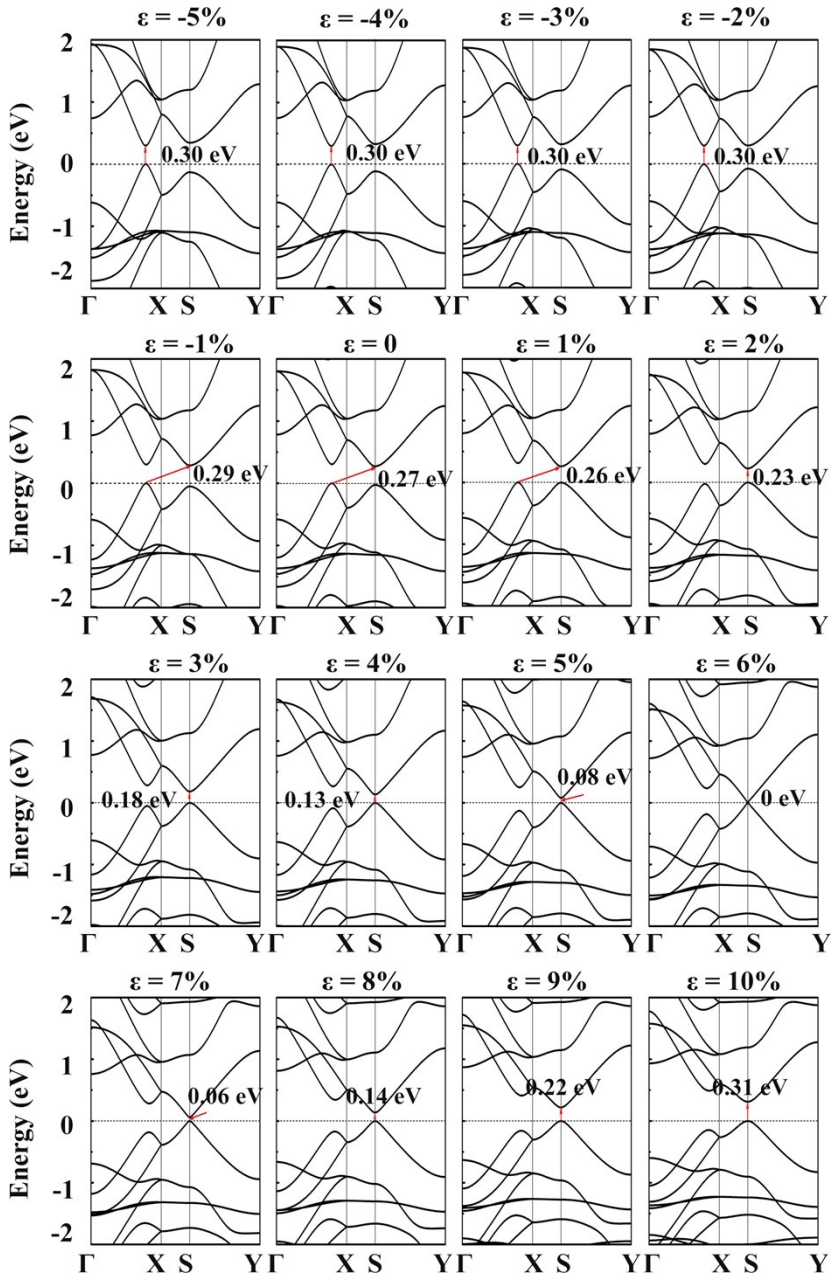

Figure S3. Electronic band structures of naphyne under the biaxial tensile strain from 1-10 %.

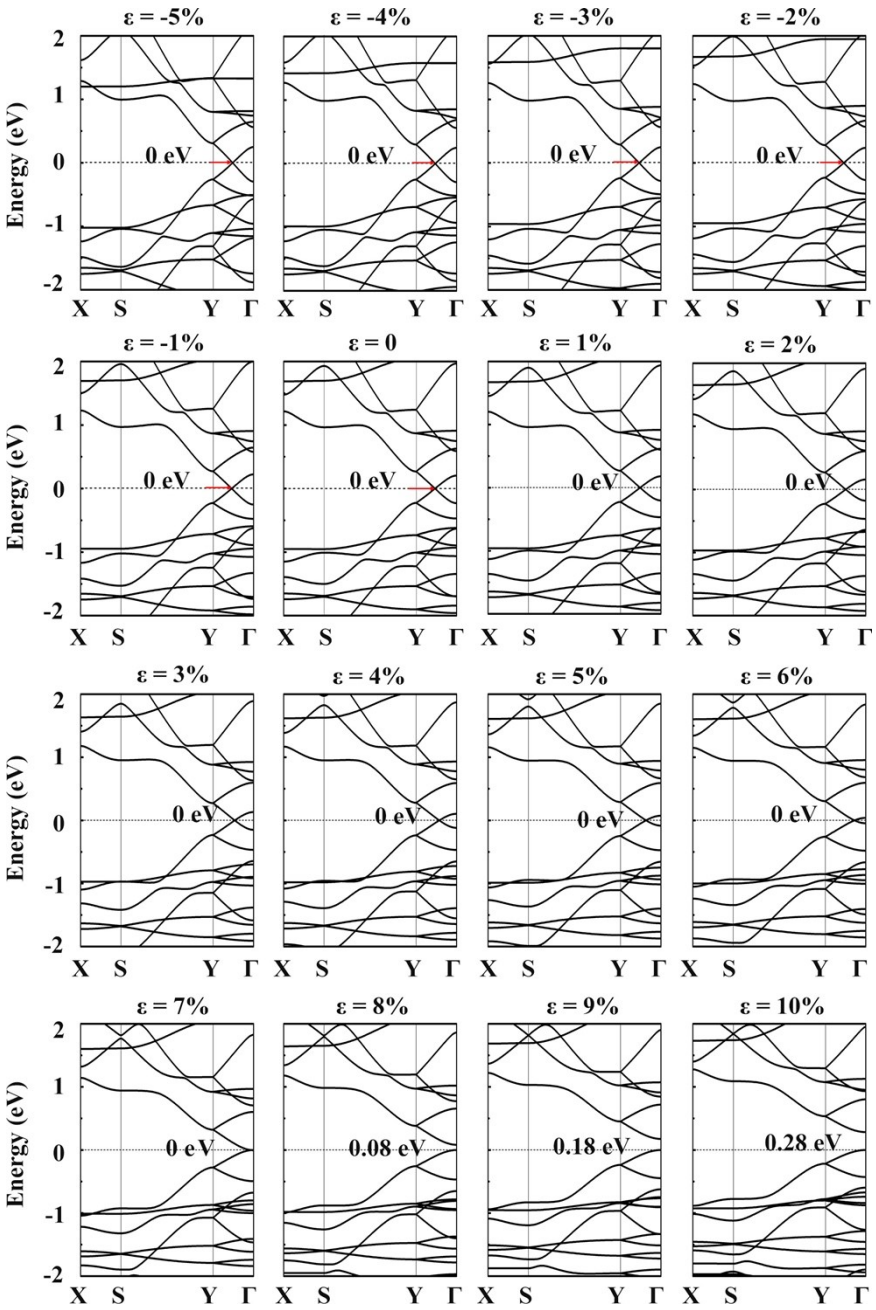

Figure S4. Electronic band structures of naphthaldiyne under the biaxial tensile strain from 1-10 %.