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

Supplementary Information

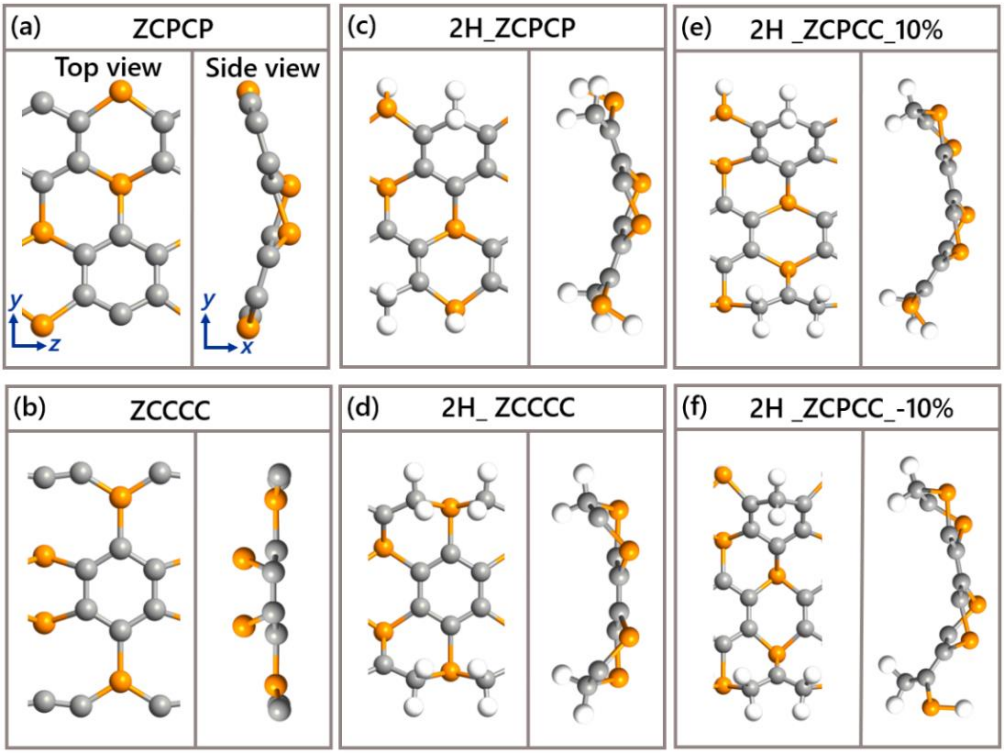

Figure S1. (a)-(b)Top and side views of ZCPCP and ZCCCC. (c)-(d) Optimized structures of ZCPCP and ZCCCC saturated with dihydrogen. (e)-(f) Optimized structures of ZCPCP saturated with dihydrogen at 10% tensile and -10% compressive strain.

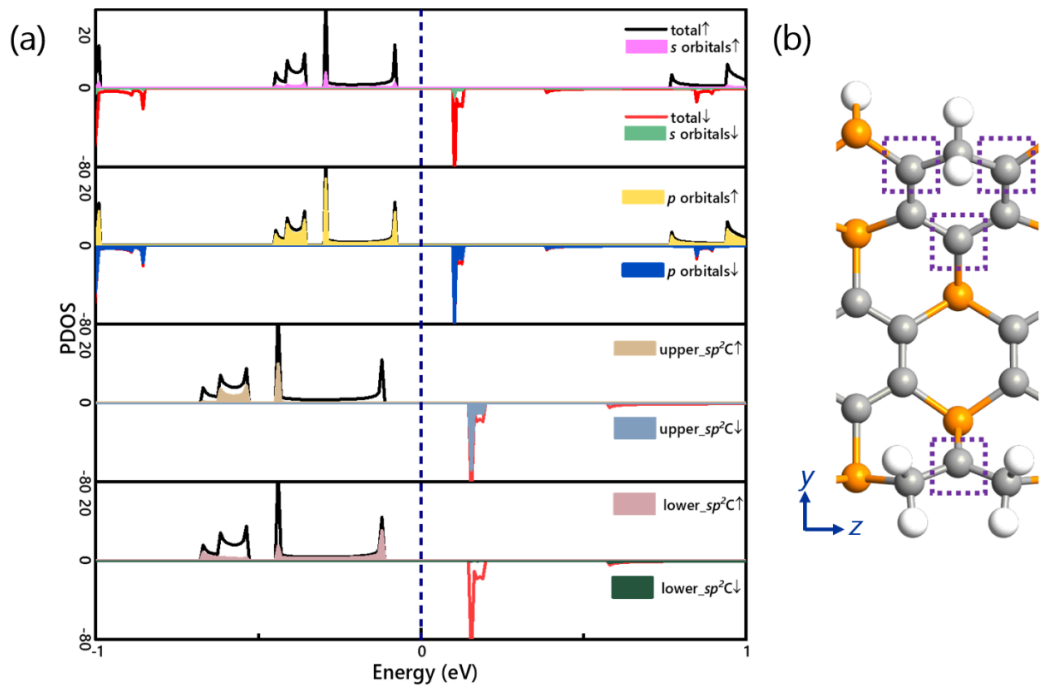

Figure S2. (a) The density of states (DOS) of the PC_3NRs system and the projected density of states (PDOS) of *s* orbitals, *p* orbitals, and C atoms with sp^2 hybridization located at the upper and lower edges. (b) Projected atoms are marked with purple rectangles. Up and down arrows indicate spin-up and down.

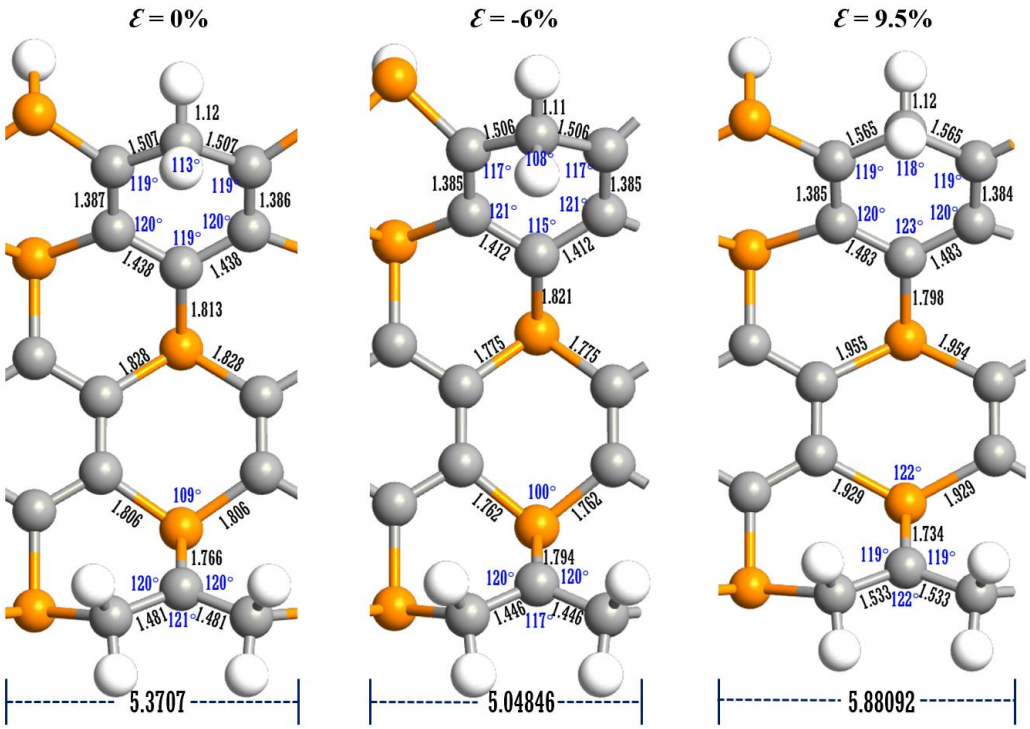

Figure S3. Bond lengths, bond angles and lattice constants of PC_3NRs at no strain, -6% compressive strain and 9.5% tensile strain. Length is expressed in Å.

Table S1. The energy differences between the FM and AFM states

	(eV/atom)		
ε	**FM**	**AFM**	**ΔE**
-10%	-6.96640	-6.96635	-0.00005
-9%	-6.99429	-6.99433	0.00004
-7%	-7.04207	-7.04211	0.00004
-6%	-7.06139	-7.06150	0.00011
-5%	-7.07028	-7.07835	0.00807
-3%	-7.10306	-7.10330	0.00024
0%	-7.12036	-7.12044	0.00008
3%	-7.11481	-7.11525	0.00044
5%	-7.09944	-7.10018	0.00074
7%	-7.07556	-7.07682	0.00126
9%	-7.04472	-7.04682	0.00210
9.5%	-7.03618	-7.03861	0.00243
10%	-7.02728	-7.02985	0.00257

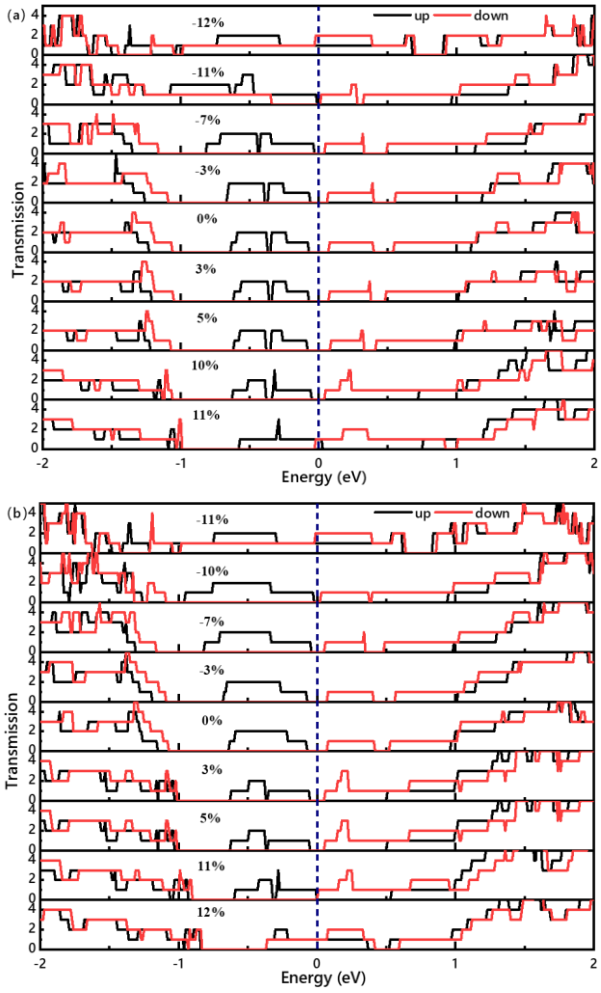

Figure S4. (a)-(b) Spin-dependent transmission spectra of PC_3NRs with widths of 7 and 9 under uniaxial strain, respectively. Black/red solid lines indicate spin up/down.

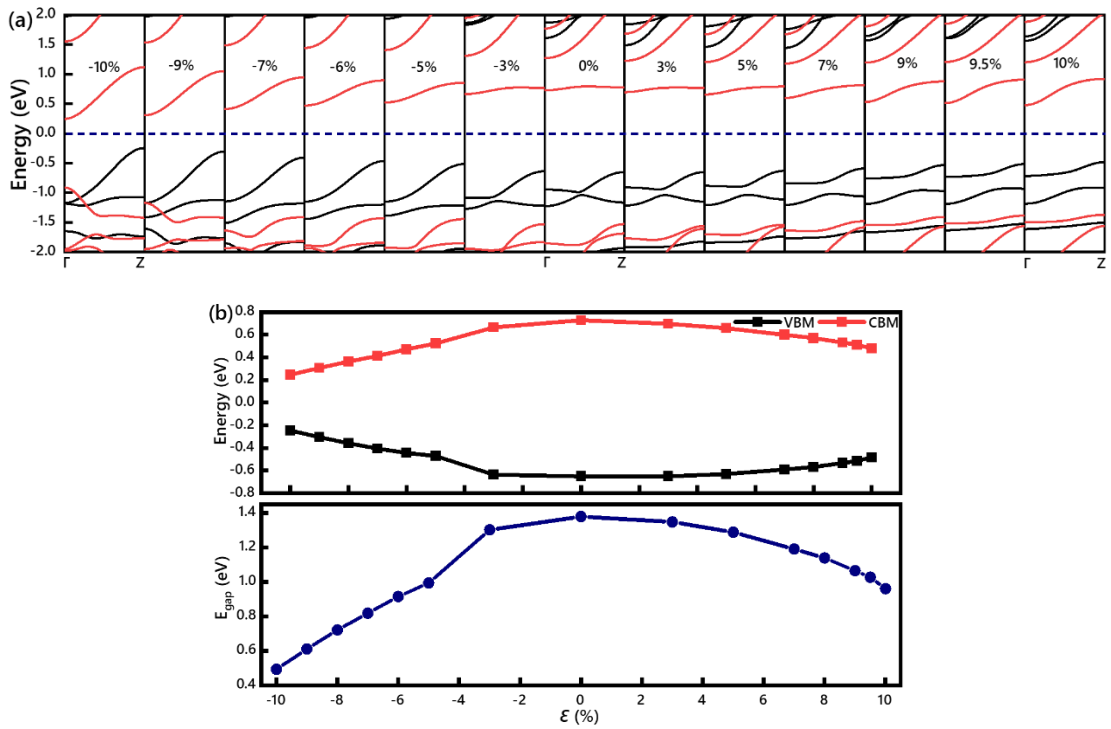

Figure S5. (a) Band structure of PC_3NR under different uniaxial strains calculated using HSE. The black/red solid lines indicate the up/down spin. (b) CBM, VBM and bandgap variation trends under uniaxial strain.