Electronic Supplementary Material (ESI) for RSC Advances.
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Contrastive band gap engineering of strained graphyne nanoribbon with armchair and zigzag edges

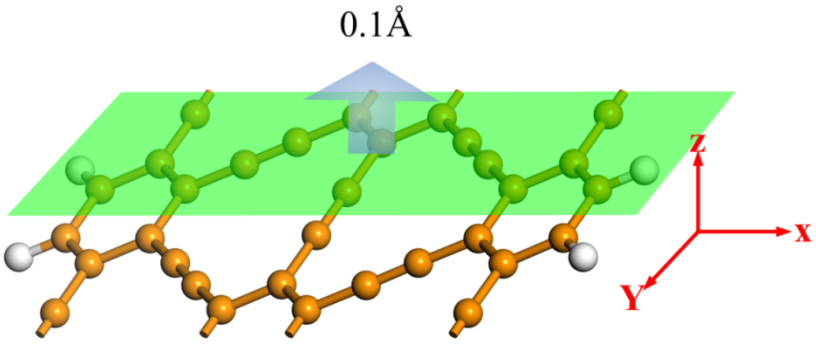

Figure S1 schematic of initial buckling or undulation, out-of-plane atom movement by hand

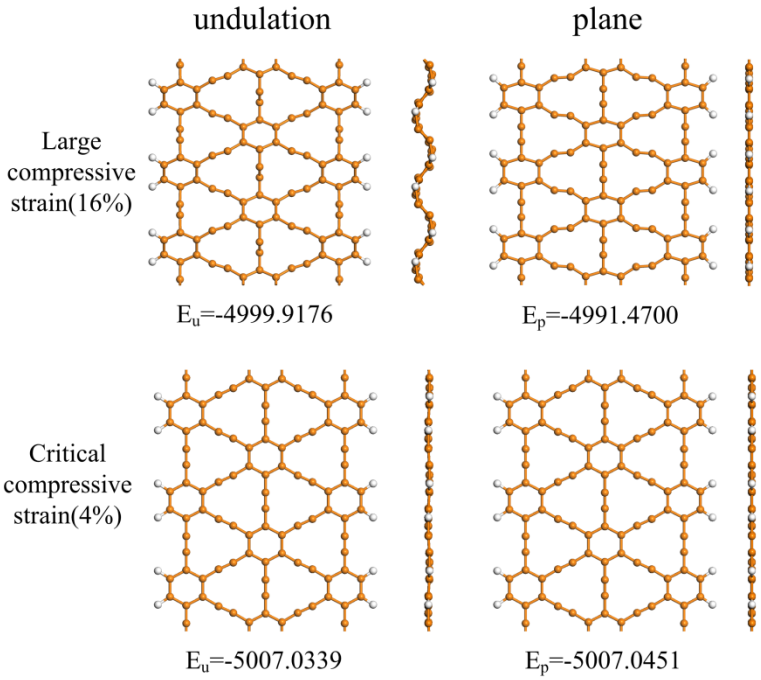

Figure S2 The energy and structure of GNR (n=3) under large and critical compressive strain.

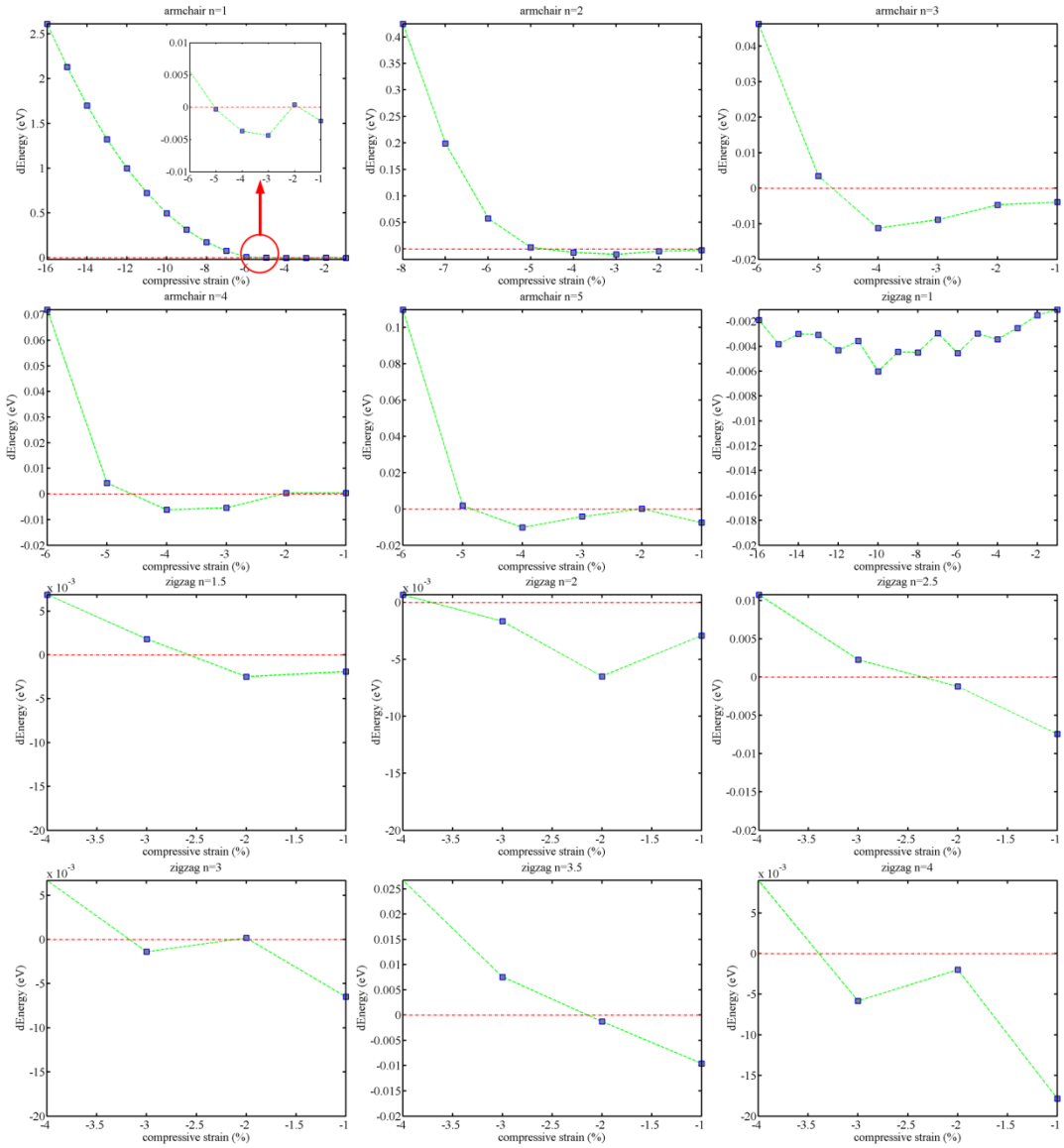

Figure S3 The dEnergy (difference value of energy with two initializations) variation as compressive strain decreases.

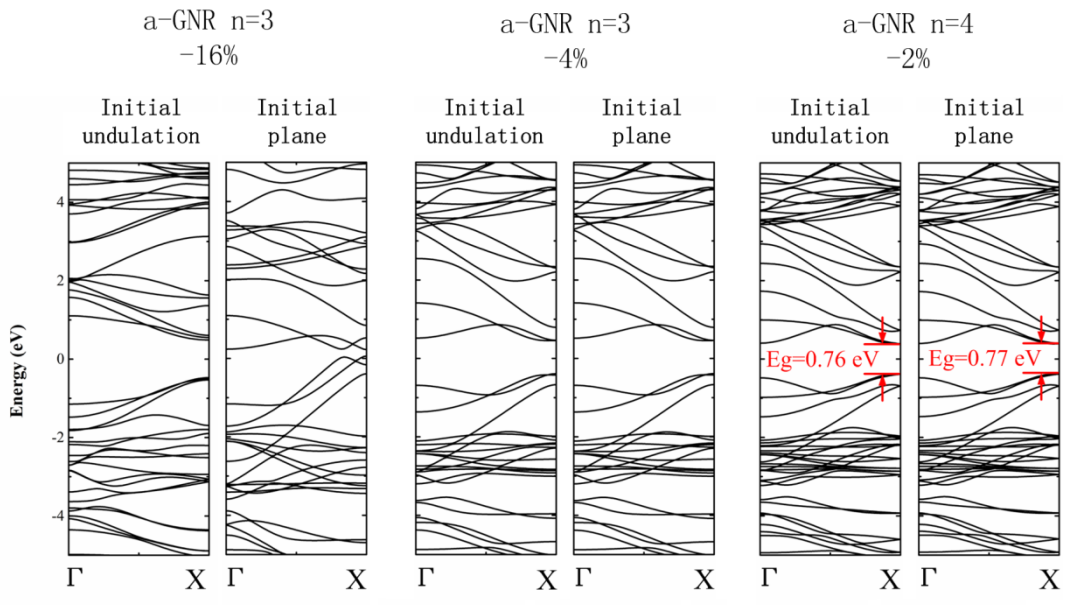

Figure S4 the band structures of GNRs with different initialization, widths and compressive strain. Under large compressive strain, electronic properties and band structures are completely different. On contrary, as strain decrease to chosen range, the energy of two different initial structures is very close, and the band structures are very similar, indicating that under appropriate compressive strain, GNRs would not wrinkle automatically and have electronic property of plane structure.

Table RI The critical compressive strain of GNRs

a-GNR n=1	**a-GNR n=2**	**a-GNR n=3**	**a-GNR n=4**	**a-GNR n=5**	**z-GNR n=1**
5%	4%	4%	4%	4%	16%
z-GNR n=1.5	**z-GNR n=2**	**z-GNR n=2.5**	**z-GNR n=3**	**z-GNR n=3.5**	**z-GNR n=4**
2%	3%	2%	3%	2%	3%