

Supporting Information

## Flexible Structural and Electronic Properties of a Pentagonal B<sub>2</sub>C Monolayer via External Strain: A Computational Investigation

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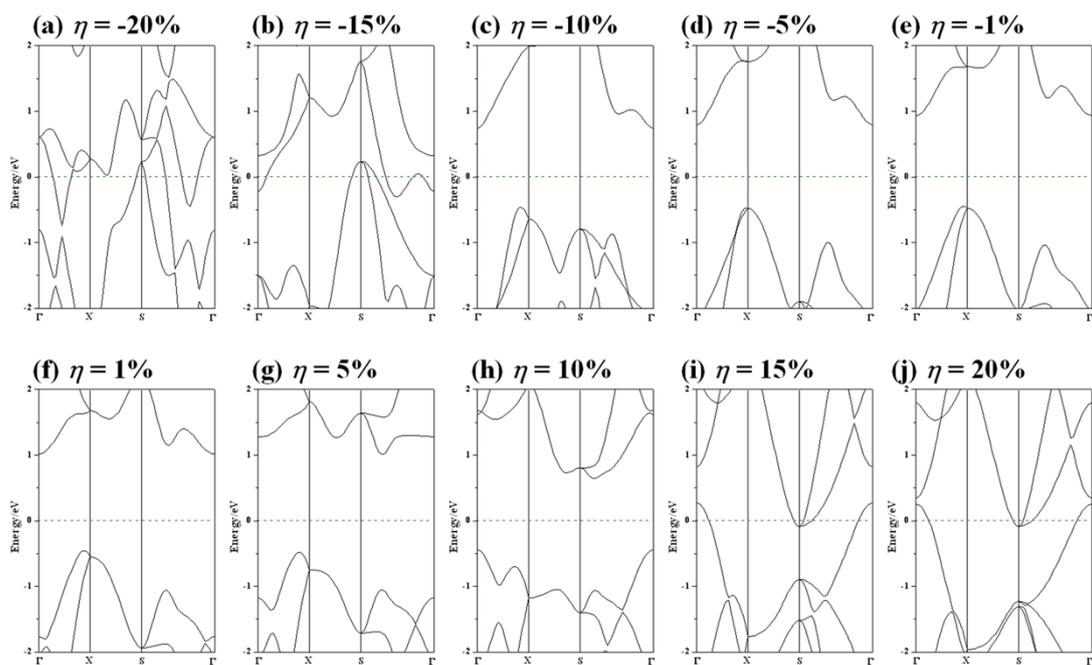
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(Z.C.)

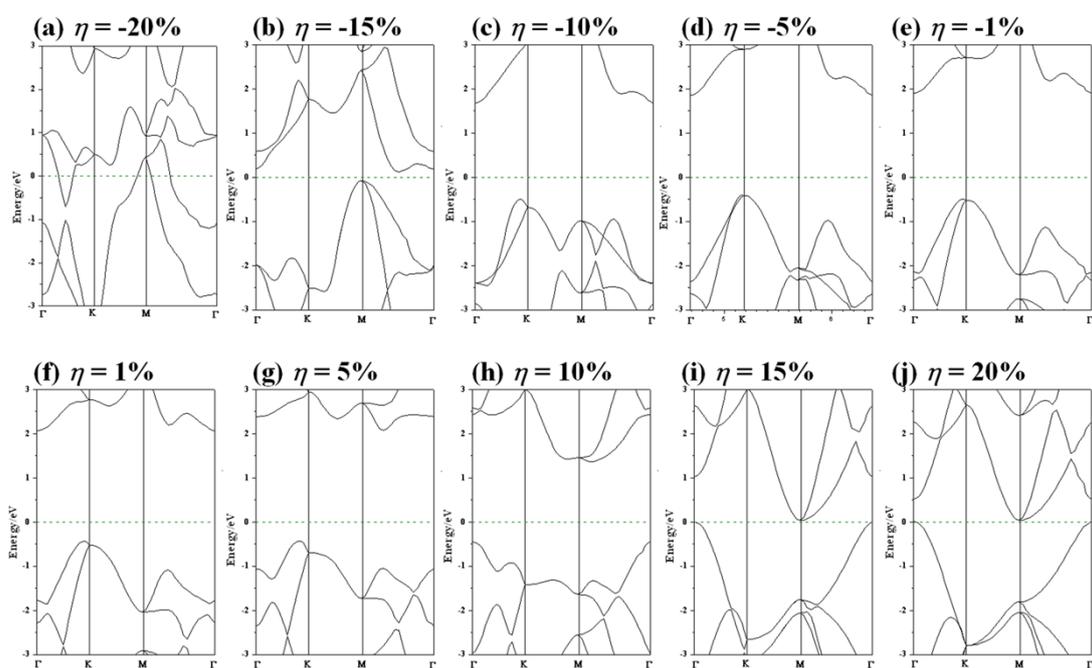
**Table S1** Structural parameters and band gaps ( $E_{\text{gap}}$ ) of biaxial strained pentagraphene monolayer,  $h$  denotes the thickness of the buckled penta-C monolayer, and  $d$  represents the average bond length.

	$h/\text{\AA}$	$d_{\text{C1-C2}}/\text{\AA}$	$d_{\text{C2-C2}}/\text{\AA}$	$\theta_{\text{C2C1C2}}/^\circ$	$\theta_{\text{C1C2C2}}/^\circ$	$\theta_{\text{C1C2C1}}/^\circ$	$E_{\text{gap}}/\text{eV}$
$\eta = -17\%$	1.73	1.43	1.36	111	106	97	0.98
$\eta = -15\%$	1.66	1.44	1.35	109	107	99	1.91
$\eta = -10\%$	1.51	1.47	1.33	105	110	104	2.55
$\eta = -5\%$	1.36	1.51	1.33	102	112	108	3.08
$\eta = 0\%$	1.21	1.55	1.34	99	113	112	3.28 (3.25 <sup>a</sup> )
$\eta = 5\%$	1.08	1.60	1.36	97	115	115	3.38
$\eta = 10\%$	0.98	1.67	1.37	95	116	116	3.56
$\eta = 15\%$	0.90	1.74	1.38	94	117	117	3.64
$\eta = 17\%$	0.88	1.76	1.39	93	117	117	3.66

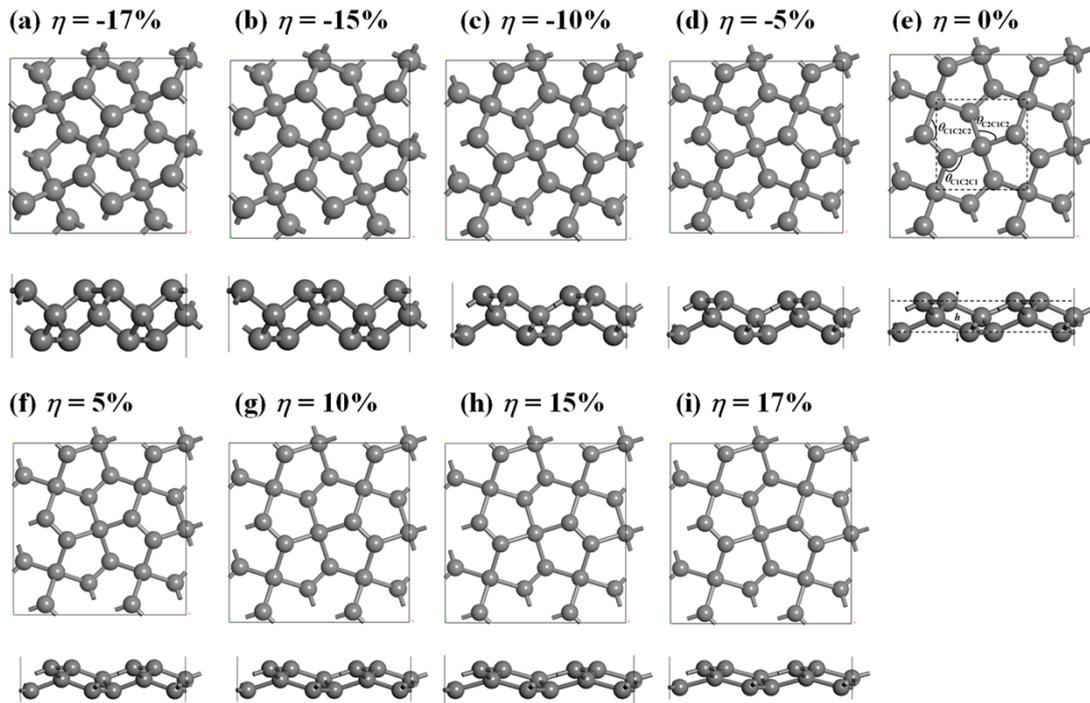
<sup>a</sup> S. Zhang, J. Zhou, Q. Wang, X. Chen, Y. Kawazoe, P. Jena, *P. Natl. Acad. Sci. USA*, 2015, **112**, 2372



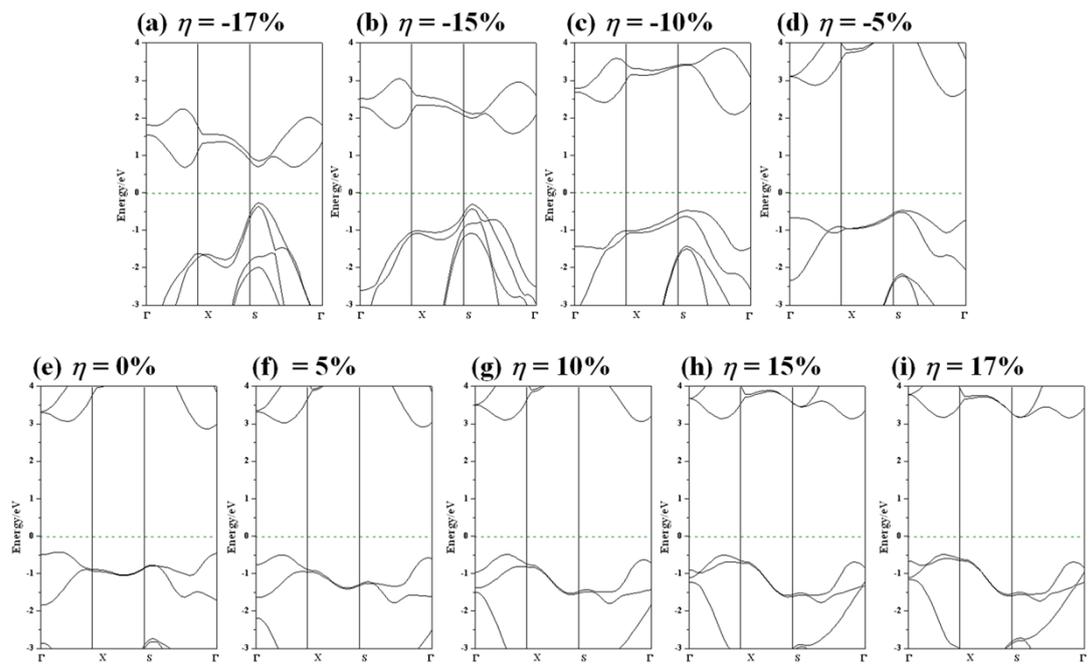
**Fig. S1** PBE band structures of penta-B<sub>2</sub>C monolayer under biaxial strain.



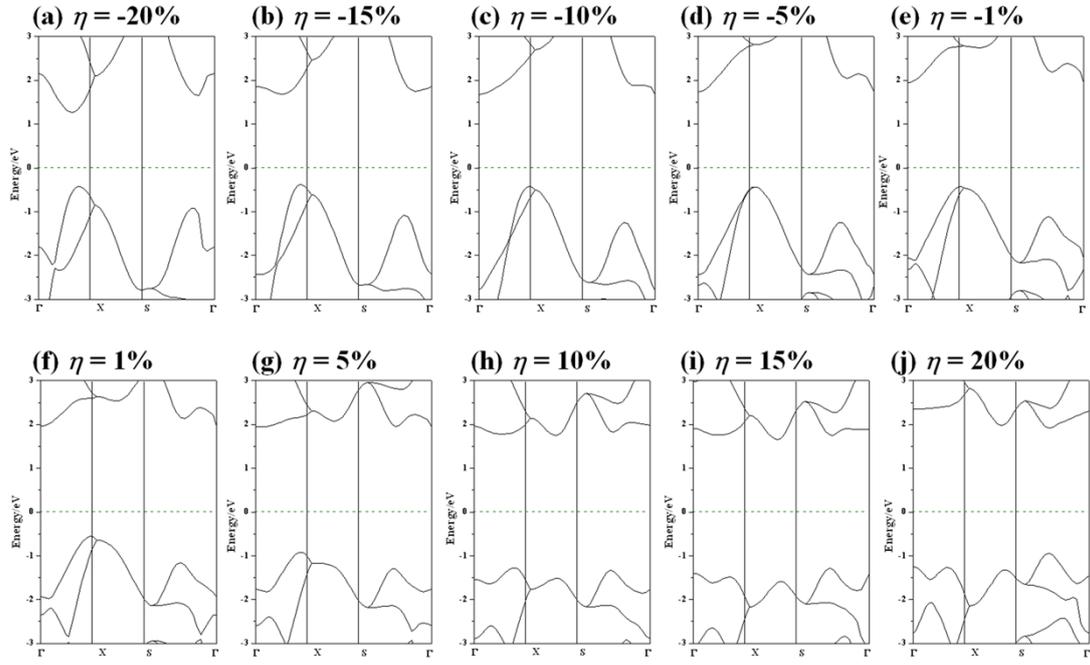
**Fig. S2** HSE06 band structures of penta-B<sub>2</sub>C monolayer under biaxial strain.



**Fig. S3** Top and side views of biaxial strained penta-graphene ( $2 \times 2$  supercell).



**Fig. S4** HSE06 band structures of penta-graphene under biaxial strain.



**Fig. S5** HSE06 band structures of penta-B<sub>2</sub>C monolayer under uniaxial strain.