Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Strain effects on stability, electronic and optical properties of two-dimensional C_4X_2 (X = F, Cl, Br)

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Table S1 Lattice constant a/b, in-plane C-C bond length $l_{C\text{-}C}$(in), interlay C-C bond length $l_{C\text{-}C}$(out), bucking height Δ and C-C-C bond angle of buckled graphene layer in the C_4X_2 (X = F, Cl, Br). The E_B is the binding energies of the C_4X_2. Length and energy units are in Å and eV/atom, respectively.

Name	a/b	$l_{C\text{-}C}$(in)	$l_{C\text{-}C}$(out)	$l_{C\text{-}X}$	Δ	θ	E_B
C_4F_2	2.560	1.561	1.547	1.369	0.503	110.126°	6.672
	2.561[1]	1.553[1]	1.553[1]	1.378[1]	0.503[1]	———	———
	2.552[2]	1.538[2]	1.556[2]	1.361[2]	0.499[2]	———	———
C_4Cl_2	2.760	1.672	1.531	1.750	0.505	111.208°	5.482
C_4Br_2	2.870	1.731	1.521	1.928	0.500	112.000°	4.966

Table S2 Average valence electrons of each C and X atoms for the C_4X_2 (X = F, Cl, Br), calculated by Bader analysis.

Name	C_1 (|e|)	C_2 (|e|)	X_1 (|e|)	C_3 (|e|)	X_2 (|e|)	C_4 (|e|)
C_4F_2	4.033	3.256	7.799	3.256	7.799	3.856
C_4Cl_2	4.089	3.884	7.119	3.844	7.119	3.903
C_4Br_2	4.039	4.093	6.964	4.093	6.964	3.846

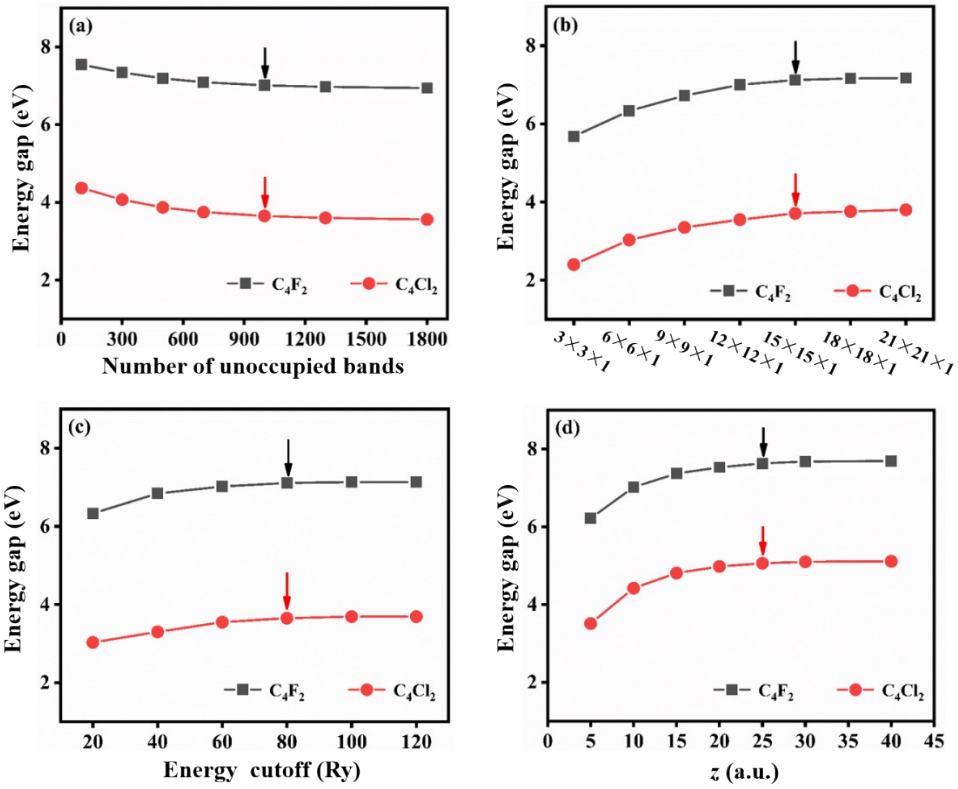

Fig. S1 Convergence of quasi-particle bandgaps with respect to the size of number of occupied bands (a), ***k***-point grid sampling of Brillouin zone (b), energy cutoff (c), and a box-shaped truncation (d) for the C_4F_2 and C_4Cl_2, respectively. The arrows denote the adopted parameters in G_0W_0 and BSE calculations.

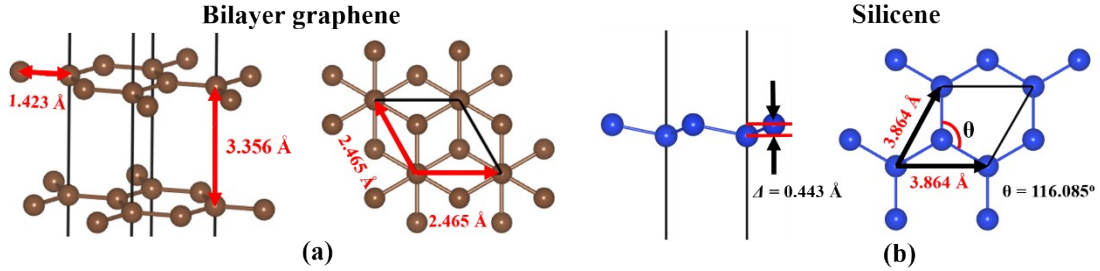

Fig. S2 Optimized geometries of the bilayer graphene (a) and silicene (b).

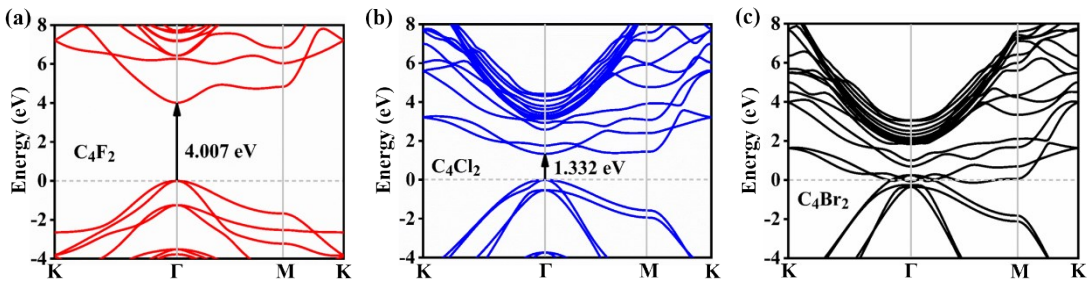

Fig. S3 Band structures of the C_4X_2 at the PBE level: (a) C_4F_2, (b) C_4Cl_2, (c) C_4Br_2.

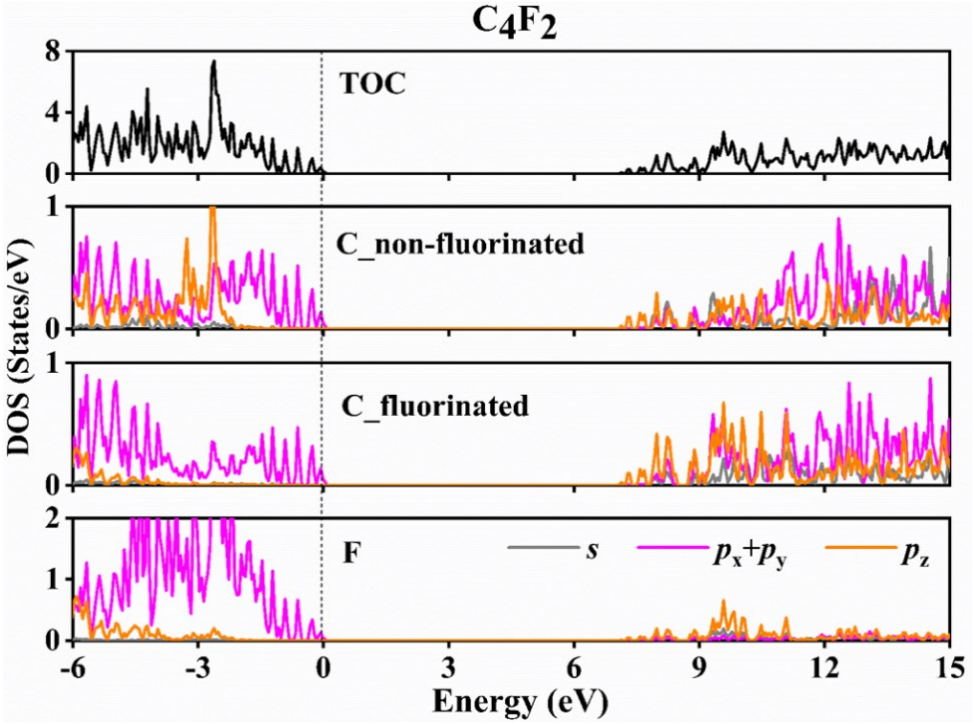

Fig. S4 Total and partial density of states of the C_4F_2. "C_fluorinated" shows the fluorinated C atoms.

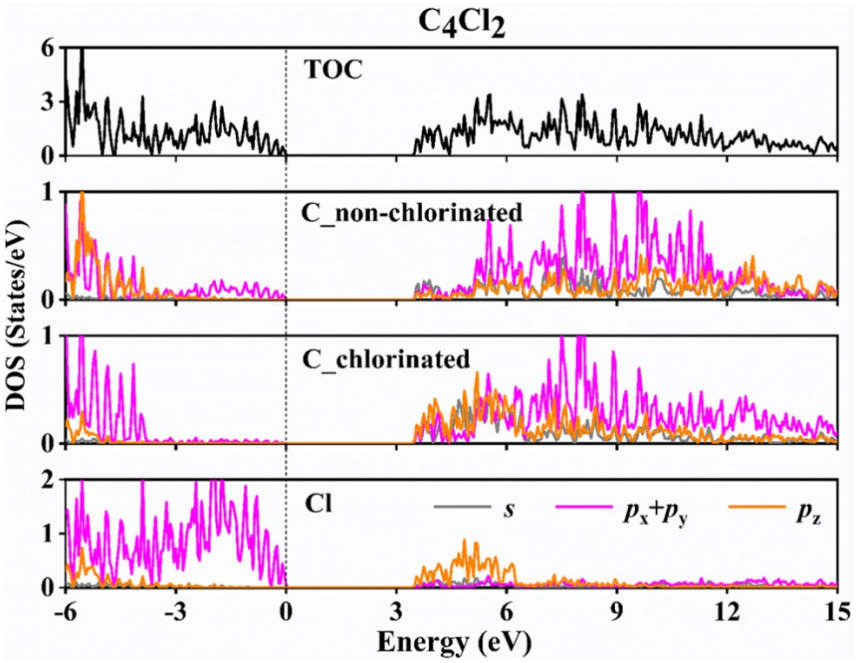

Fig. S5 Total and partial density of states of the C_4Cl_2. "C_chlorinated" shows the chlorinated C atoms.

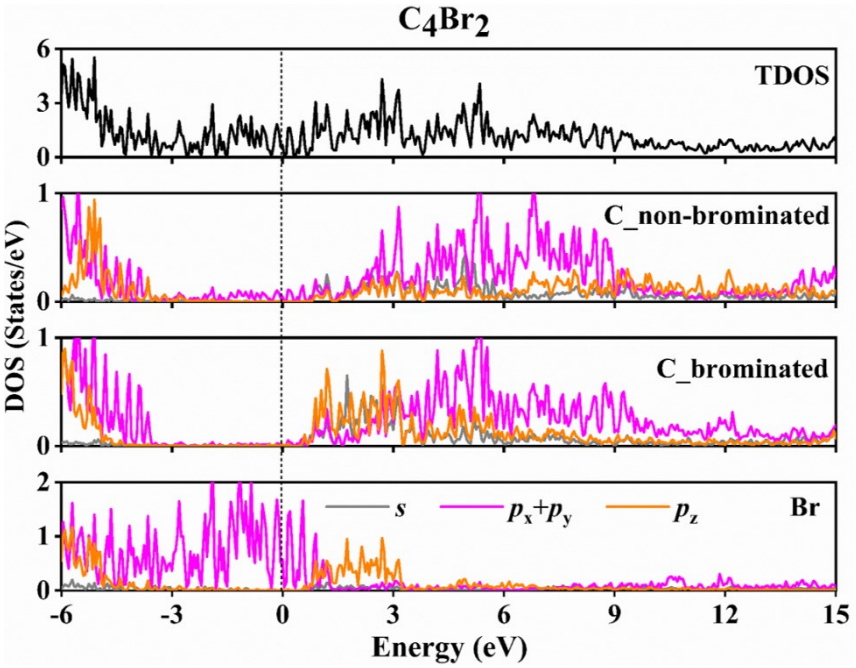

Fig. S6 Total and partial density of states of the C_4Br_2. "C_brominated" shows the brominated C atoms.

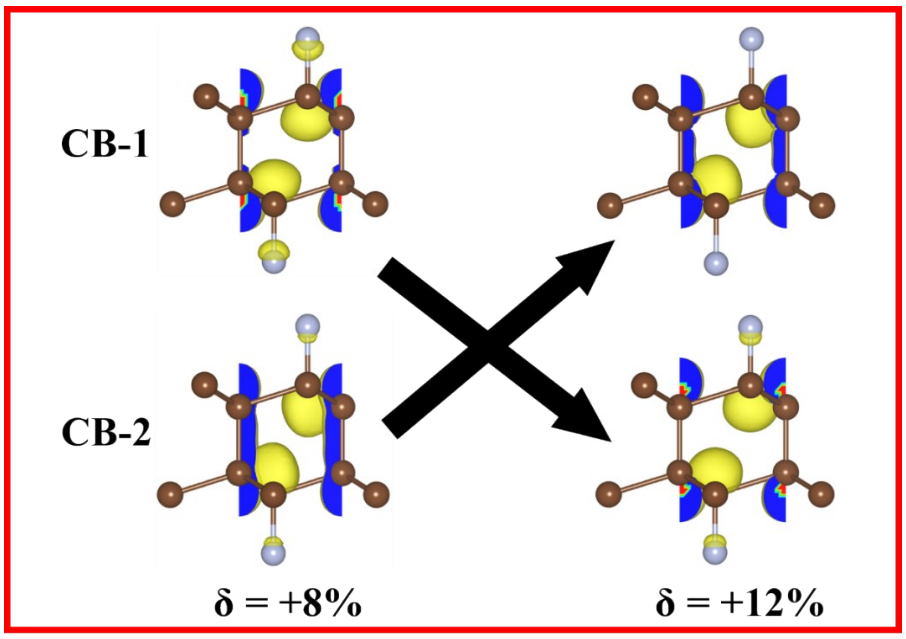

Fig. S7 Partial charge density of CB-1 and CB-2 at Γ-point for the C_4F_2 at tensile strains of 8% and 12%. Isovalue of 9×10^{-3} e/Å^3 is adopted.

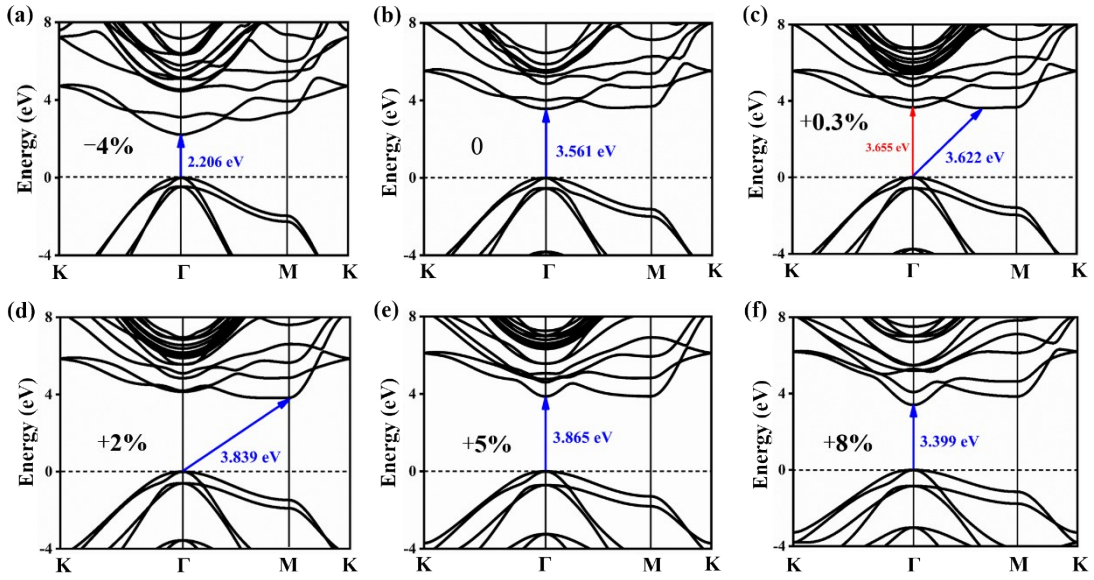

Fig. S8 (a)–(f) Variable quasi-particle band structures of the C_4Cl_2 under different biaxial strains (δ = −4%, 0, +0.3%, +2%, +5%, +8%).

References

1 L. Yuan, Z. Li, J. Yang and J. G. Hou, *Phys. Chem. Chem. Phys.*, 2012, **14**, 8179–8184.

2 C.-H. Hu, P. Zhang, H.-Y. Liu, S.-Q. Wu, Y. Yang and Z.-Z. Zhu, *J. Phys. Chem. C*, 2013, **117**, 3572–3579.