Electronic Supplementary Material (ESI) for RSC Advances.

Electronic supplementary information

Ideal strength and elastic instability in single-layer 8-*Pmmn* Borophene

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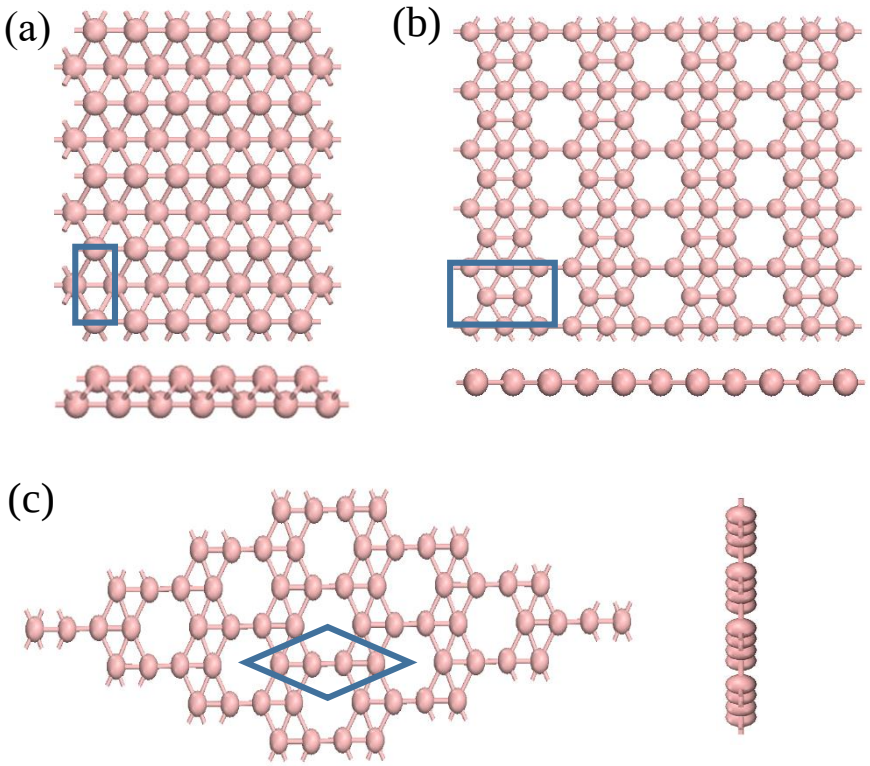
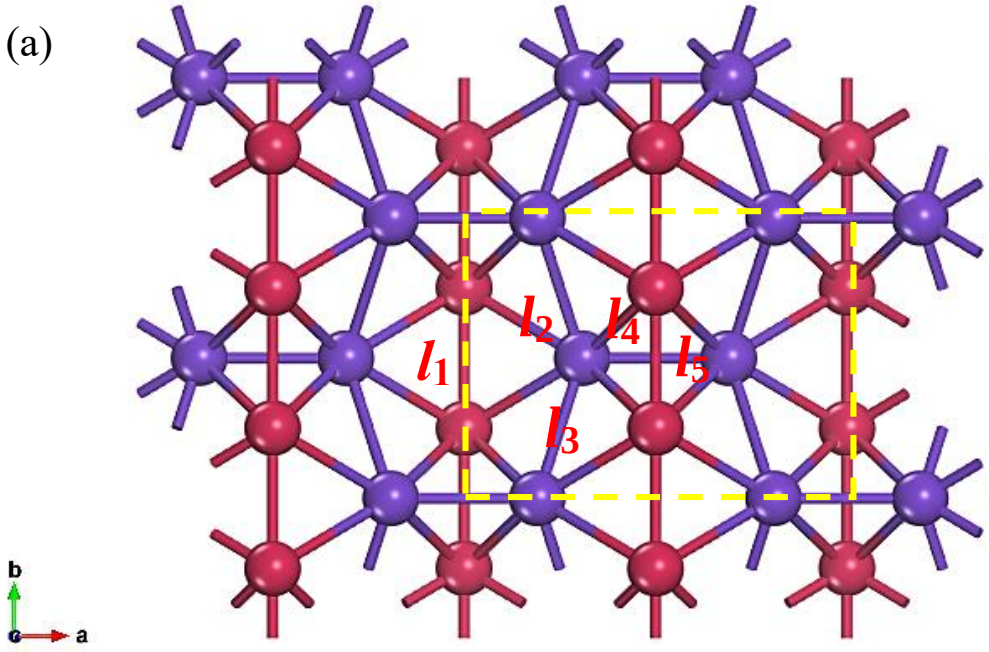


Fig. ESI1 Top view and side view of (a) striped, (b) β_{12} and (c) χ_3 borophene.

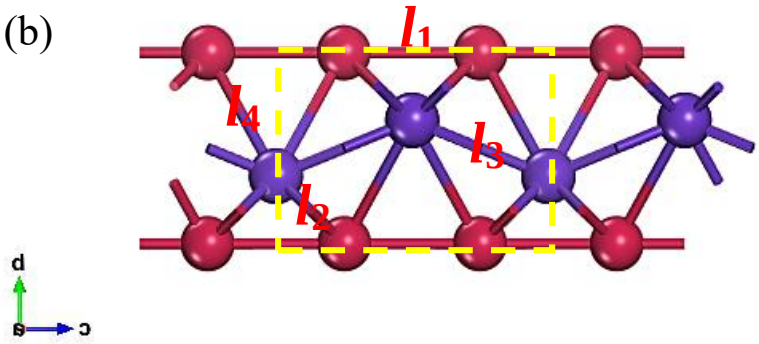
Table ESI1 Calculated lattice constant *a* and *b*, buckling height *h*, and energy *E* of 8-*Pmmn*, stripe, β_{12} and χ_3 borophene. Previous theoretical data are also listed for comparison.

Structure	*a* (Å)	*a* (Å)	*h* (Å)	*E* (eV/atom)	*Ec* (eV/atom)
8-*Pmmn* borophene	4.523	3.258	2.18	-6.325	-6.038
Ref. 1	4.52	3.26	--	-6.394	--
stripe borophene	1.614	2.868	0.907	-6.187	-5.900
β_{12} borophene	5.070	2.928	0	-6.232	-5.945
χ_3 borophene	4.459	4.459	0	-6.244	-5.957
stripe borophene [13]	1.614	2.866	0.911	--	-6.099
stripe borophene [1]	1.61	2.87	--	-6.242	--
β_{12} borophene [13]	5.07	2.93	0	--	-6.147
β_{12} borophene [1]	5.08	2.92	--	-6.282	--
χ_3 borophene [13]	4.45	4.45	0	--	-6.159

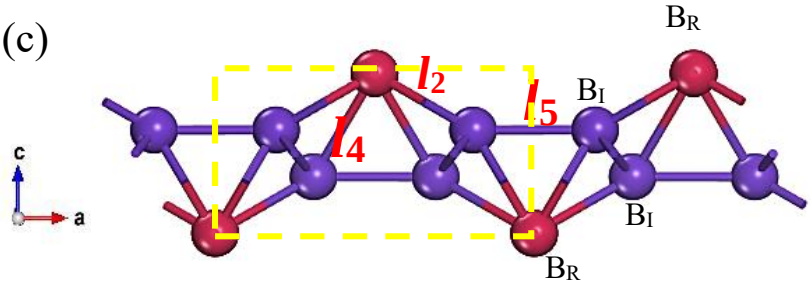
(a)



(b)



(c)



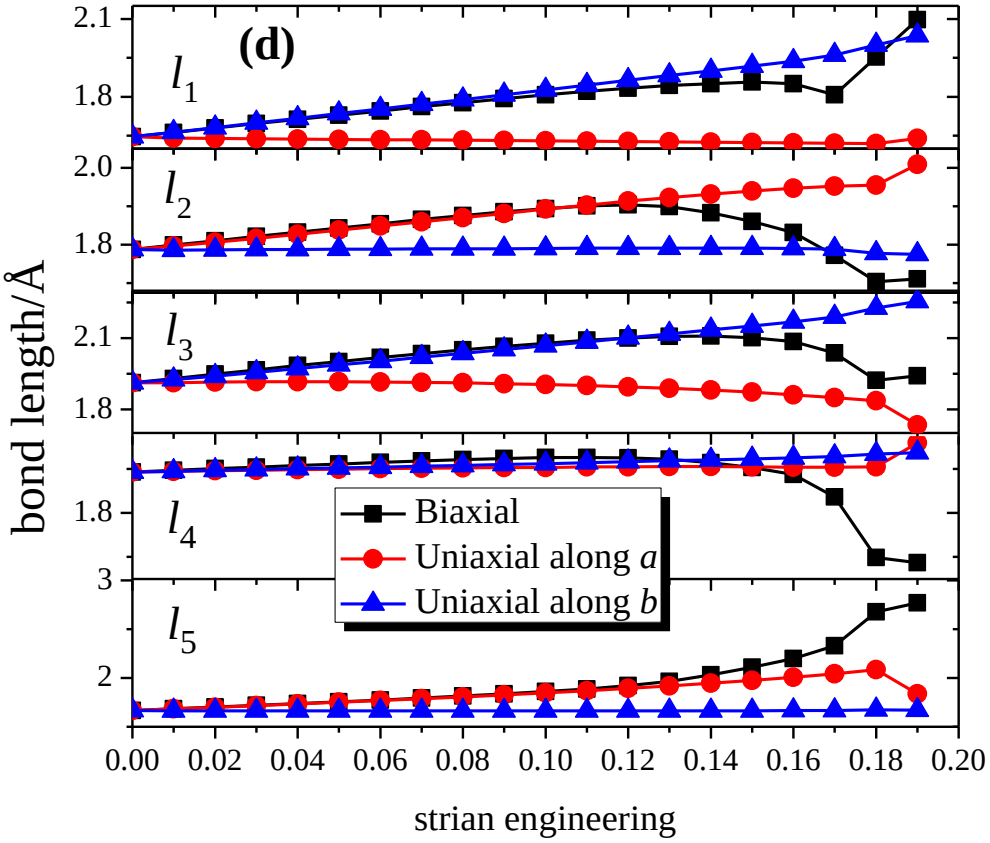
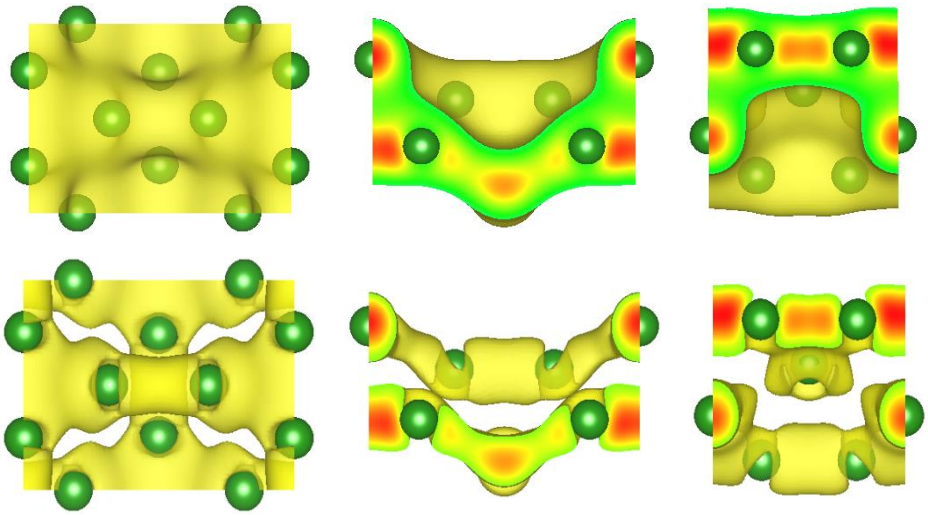
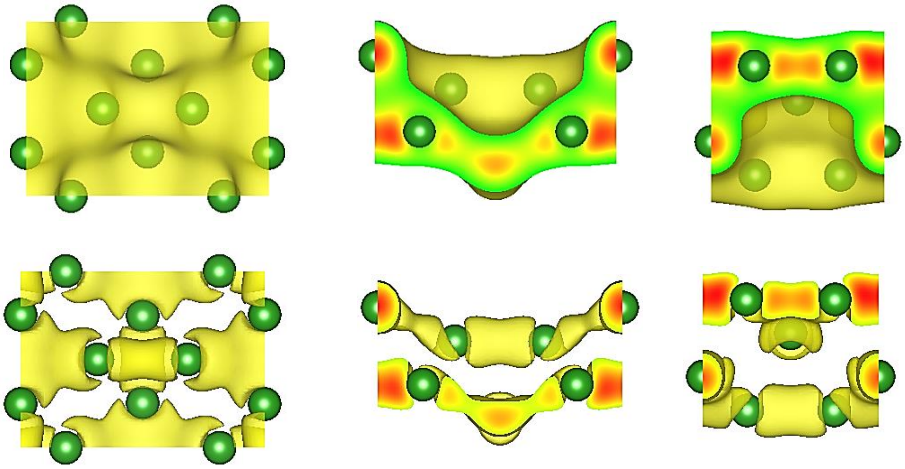


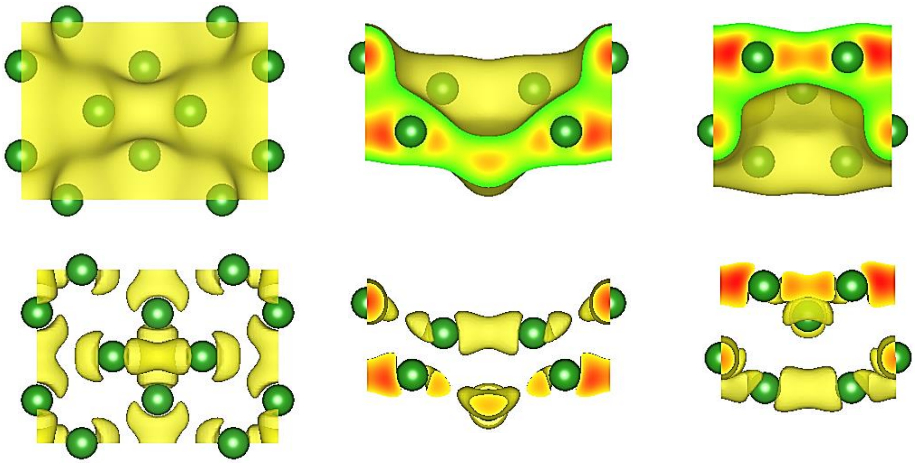
Fig. ESI2 The calculated bond length of 8-*Pmmn* borophene. The five types B-B bonds (l_1, l_2, l_3, l_4 l_5) are shown in Fig.ESI2 (a), (b) and (c); the corresponding B-B bond length is shown in Fig.ESI2 (d). The l_1 represent B_R-B_R bond length, l_2 and l_4 represent two different B_R-B_I bond lengths, l_3 and l_5 represent two different B_I-B_I bond lengths.



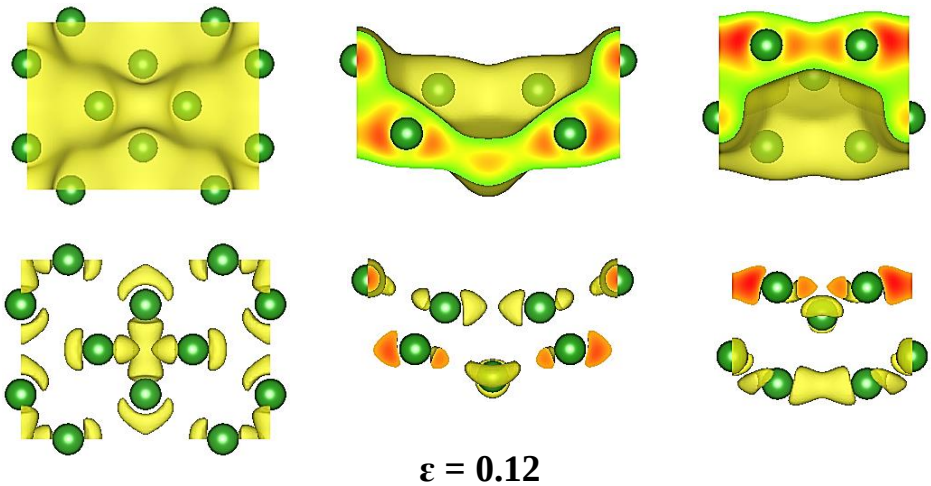
(a) **Intrinsic**



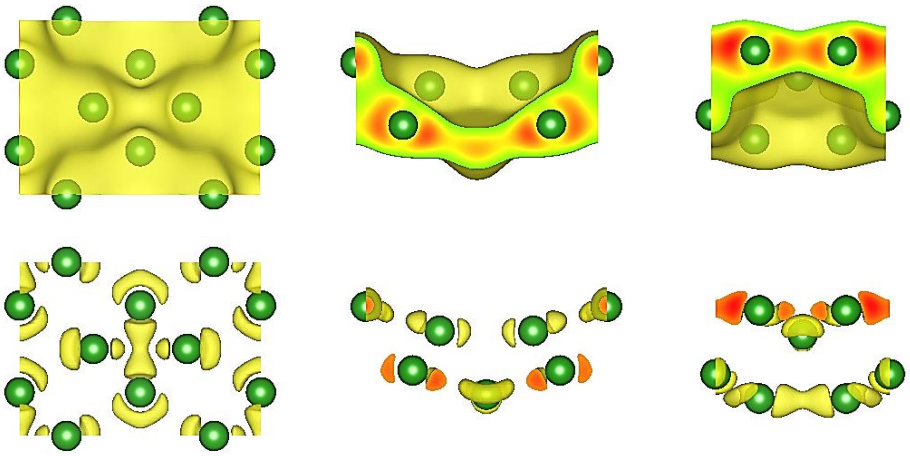
ε = 0.04



ε = 0.08

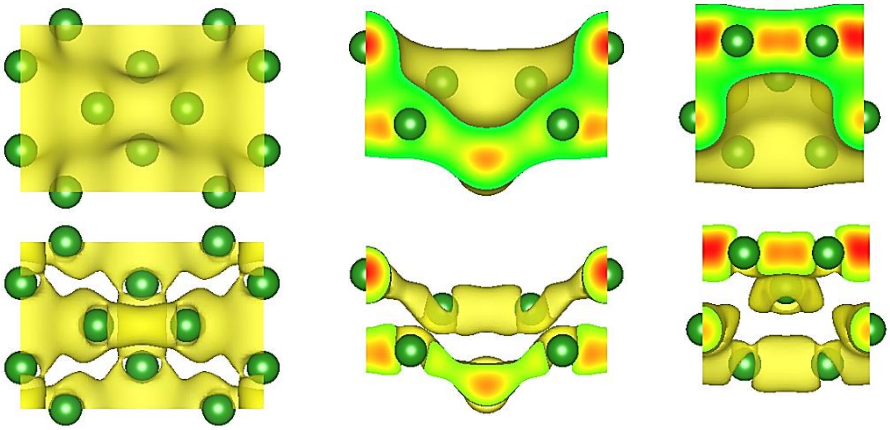


ε = 0.12

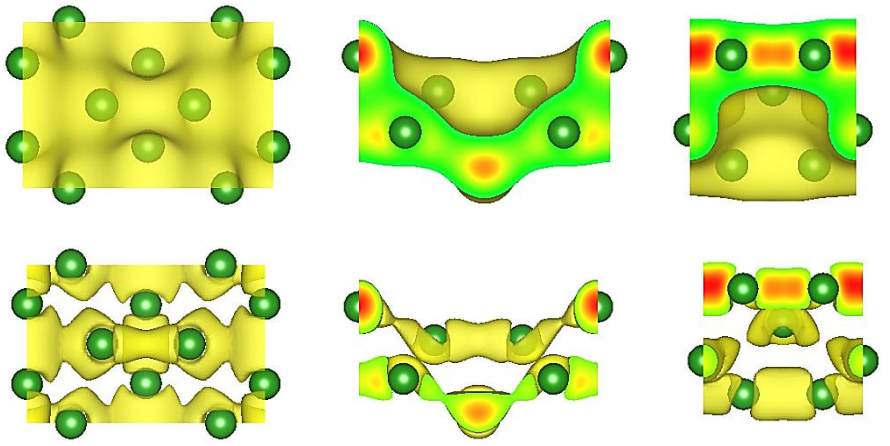


ε = 0.135

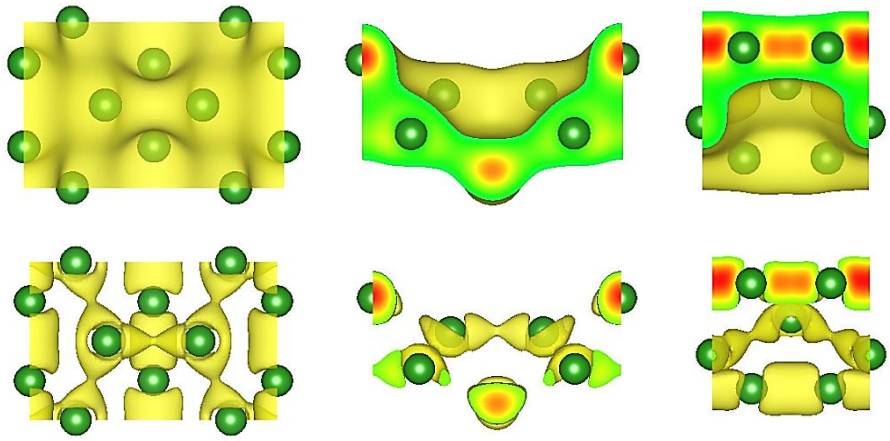
(b) Biaxial strain (ε = 0.04, 0.08, 0.12, 0.135)



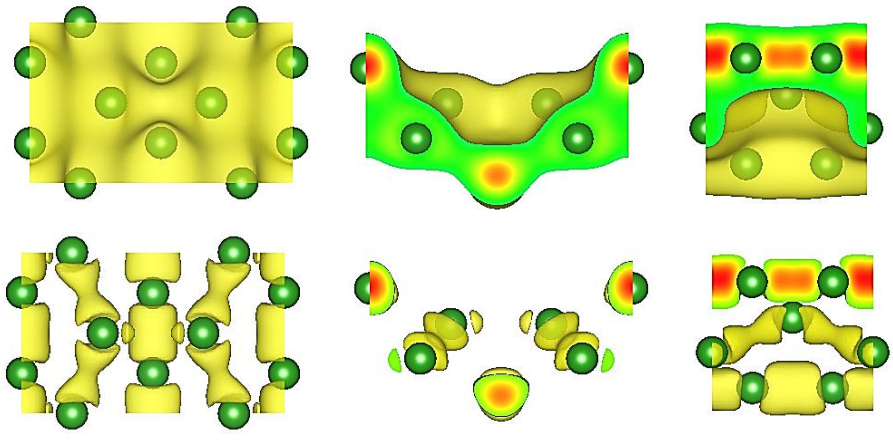
ε = 0.04



ε = 0.08

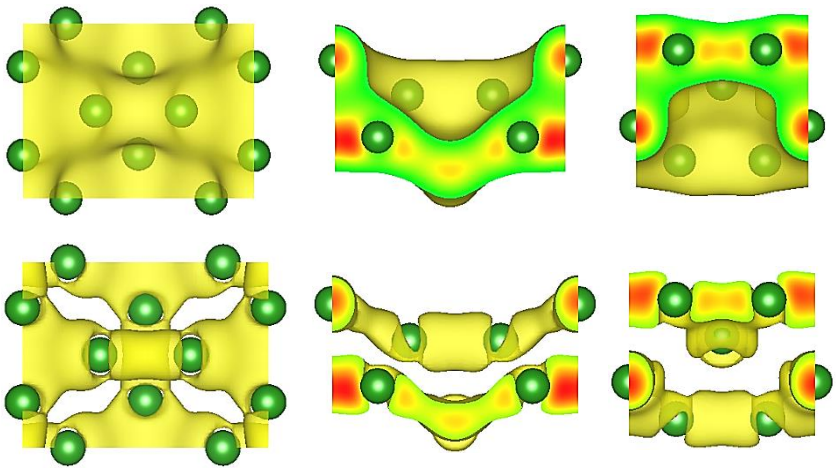


ε = 0.12

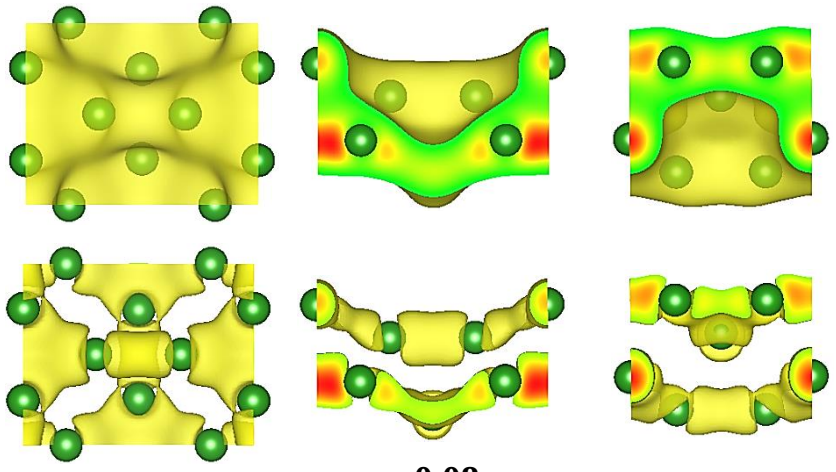


ε = 0.16

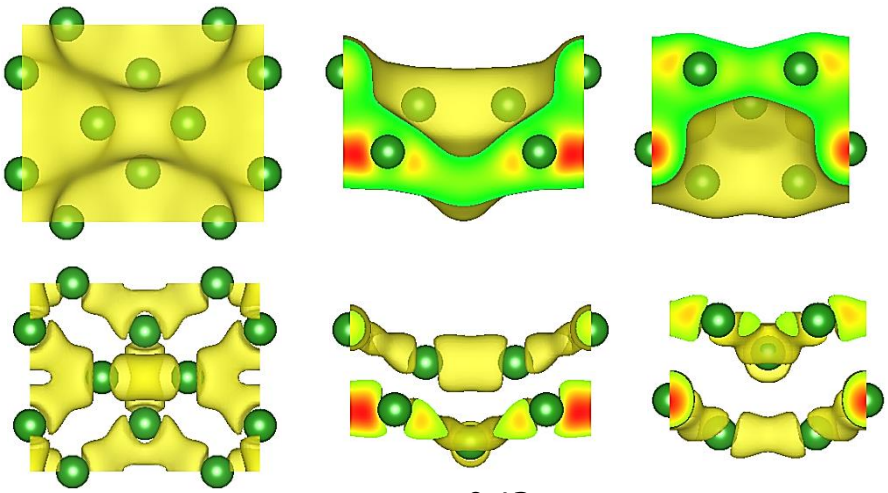
(c) Uniaxial strain along *a* (ε = 0.04, 0.08, 0.12, 0.16)



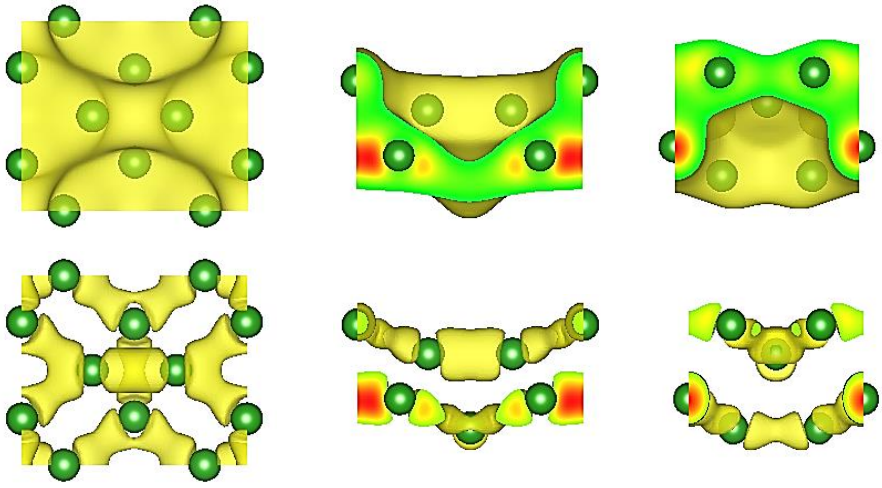
ε = 0.04



ε = 0.08



ε = 0.12



(d) Uniaxial strain along *b* (ε = 0.04, 0.08, 0.12, 0.165)

Fig. ESI3 The calculated valence electron density of 8-*Pmmn* borophene under three types of strain with two different isosurfaces. The isosurfaces of upper panel is 0.07 e/bohr^3, the lower panel is 0.10 e/bohr^3, respectively. (a) (001), (010) and (100) plane without strain; (b) (001), (010) and (100) plane under biaxial strain; (c) (001), (010) and (100) plane under uniaxial along *a* direction; (d) (001), (010) and (100) plane under uniaxial along *b* direction.

References

[1] Ma F, Jiao Y, Gao G, et al. Graphene-like Two-dimensional Ionic Boron with Double Dirac Cones at Ambient Condition[J]. Nano Letters, 2016, 16(5):3022.