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

Supplementary Information

First -Principles studies on the effects of halogen adatom adsorption on monolayer antimony.

Keat Hoe Yeoh, Tiem Leong Yoon, Duu Sheng Ong, Thong Leng Lim and Yusuf Zuntu Abdullahi

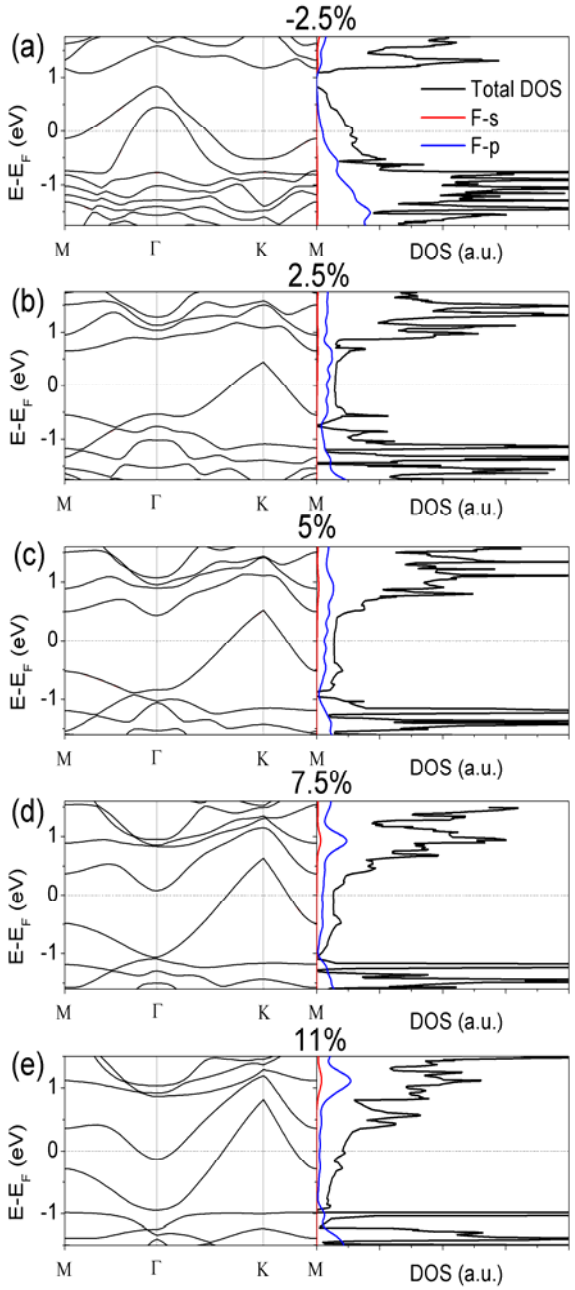

Fig S1 Band structure and DOS of β-Sb with the adsorption of F adatom under different bi-axial strain for coverage of Θ = 1/8. The projected s-states and p-states for the halogen adatoms are denoted by the red and blue respectively.

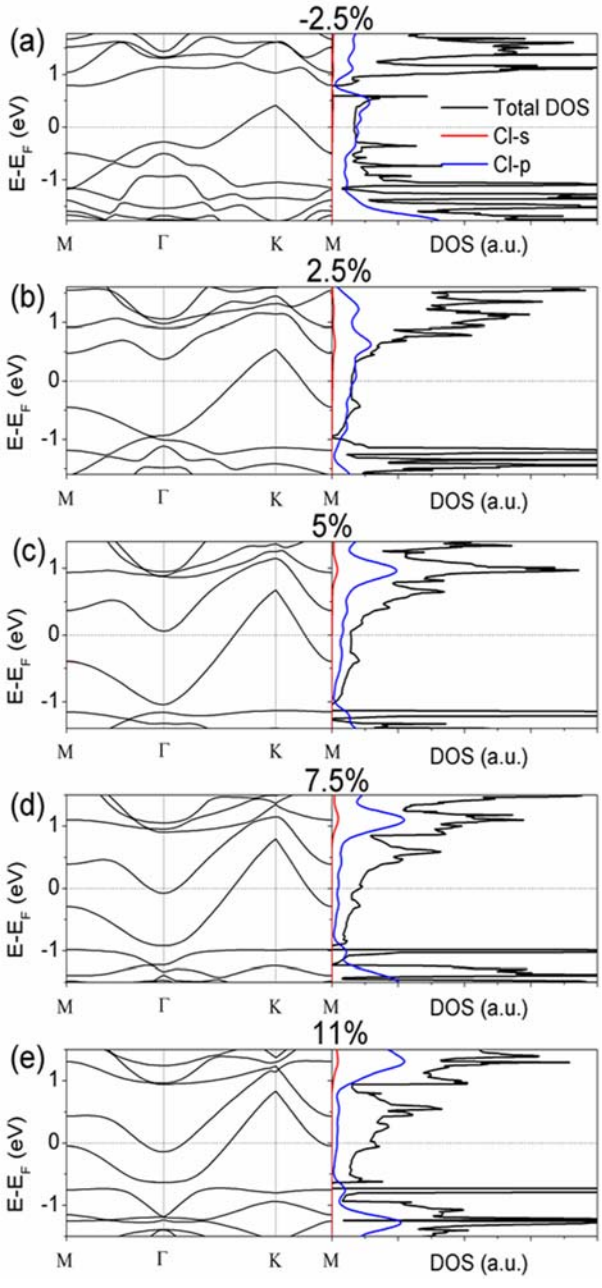

Fig S2 Band structure and DOS of β-Sb with the adsorption of Cl adatom under different bi-axial strain for coverage of Θ = 1/8. The projected s-states and p-states for the halogen adatoms are denoted by the red and blue respectively.

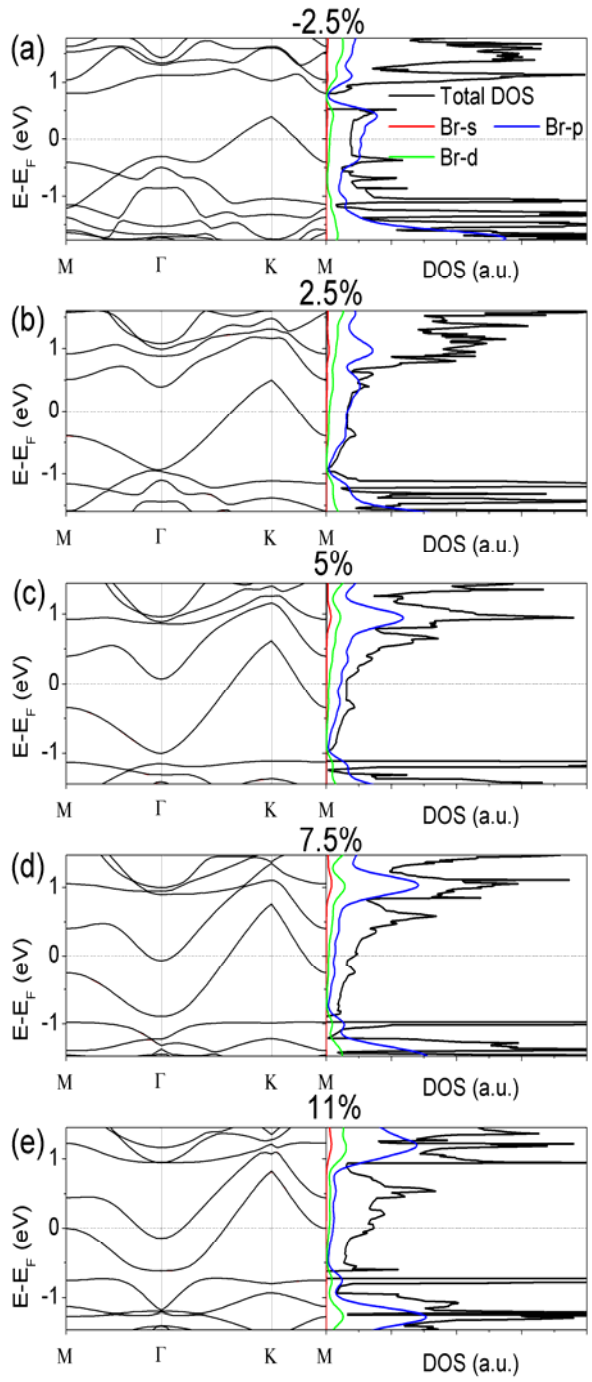

Fig S3 Band structure and DOS of β-Sb with the adsorption of Br adatom under different bi-axial strain for coverage of Θ = 1/8. The projected s-states, p-states and d-states for the halogen adatoms are denoted by the red, blue and green respectively.

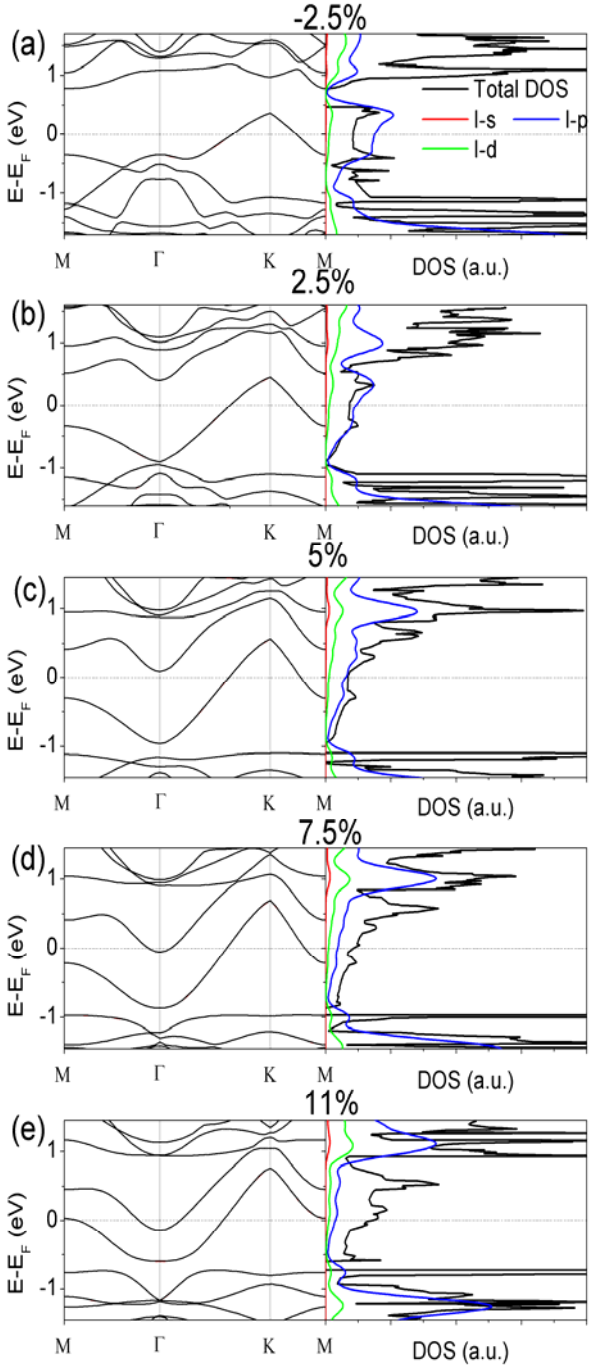

Fig S4 Band structure and DOS of β-Sb with the adsorption of I adatom under different bi-axial strain for coverage of Θ = 1/8. The projected s-states, p-states and d-states for the halogen adatoms are denoted by the red, blue and green respectively.

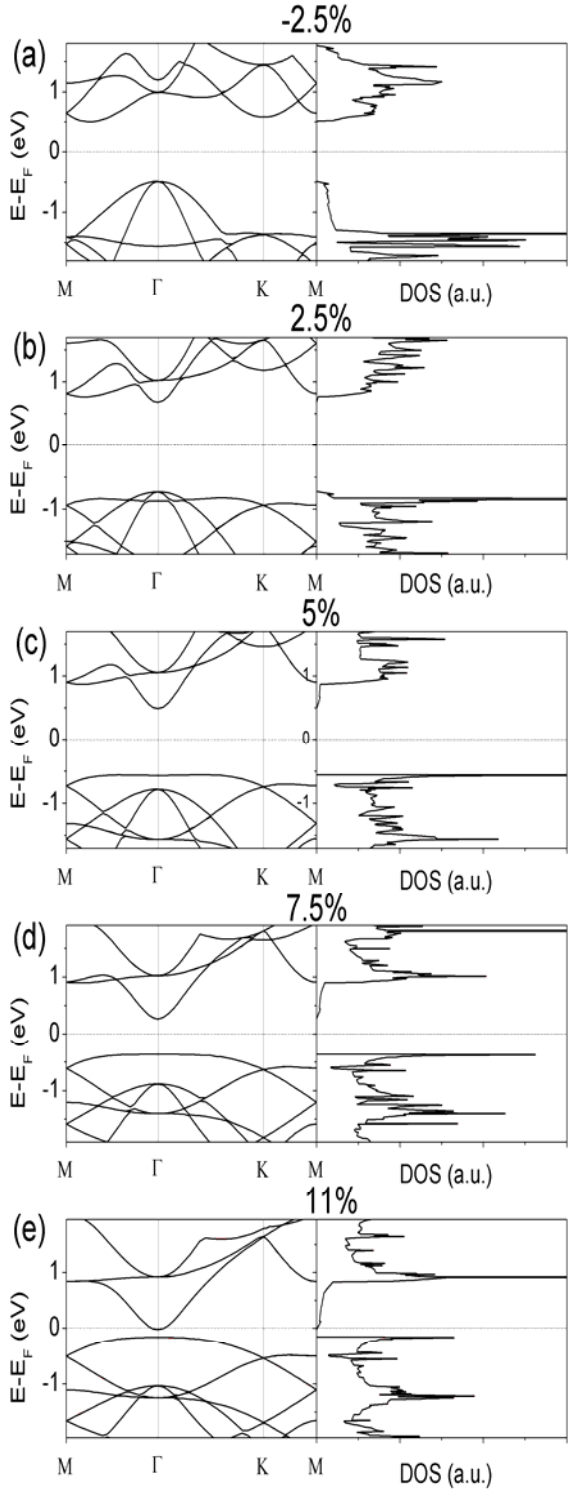

Fig S5 Band structure and DOS of pristine β-Sb under different bi-axial for a 2x2 super-cell.

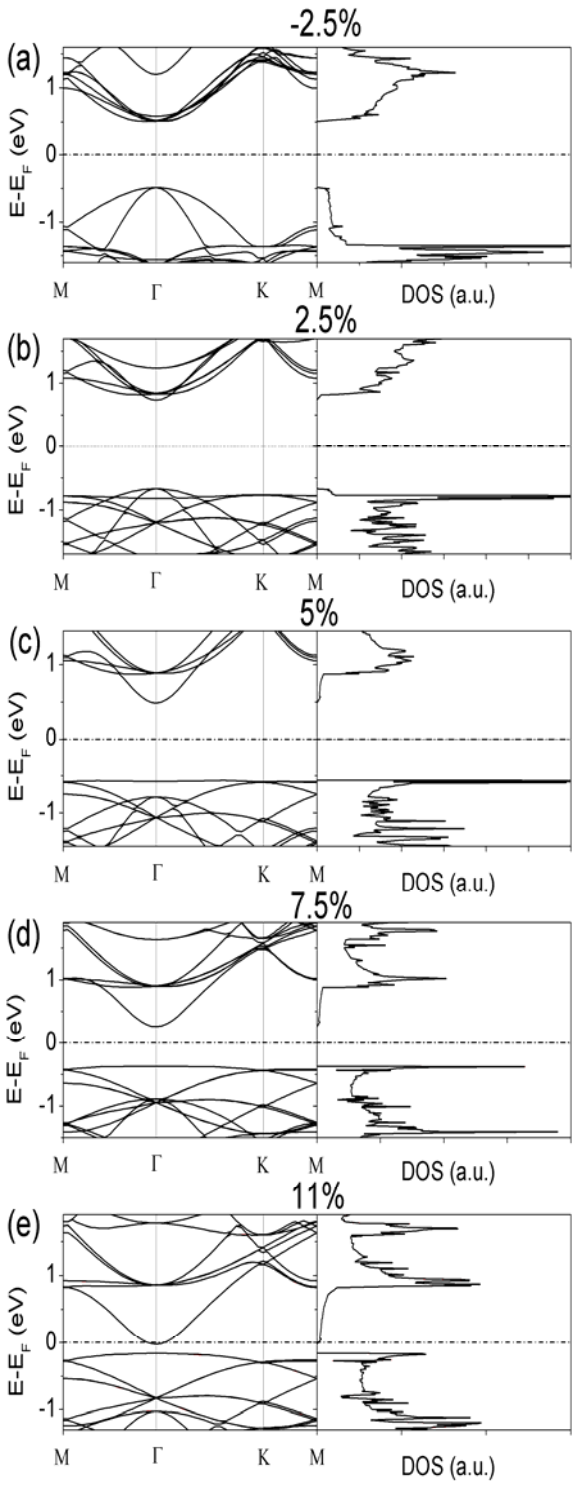

Fig S6 Band structure and DOS of pristine β-Sb under different bi-axial strain for a 3x3 super-cell.

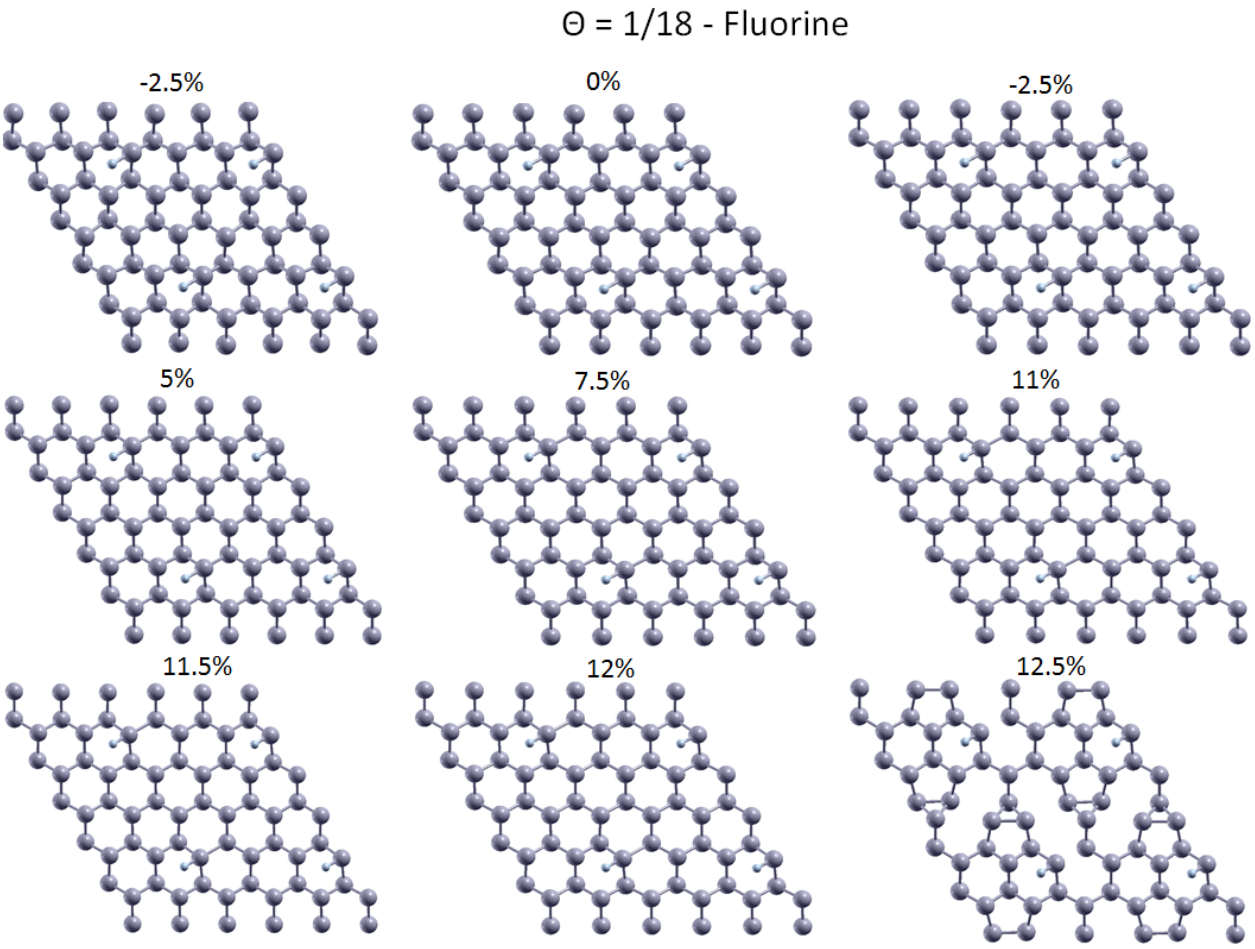

Fig S7 Top view of the most stable site for the adsorption of F for Θ = 1/18. We deliberately increased the bi-axial strain up to 12.5% where at this applied strain the β-Sb undergo structural deformation.

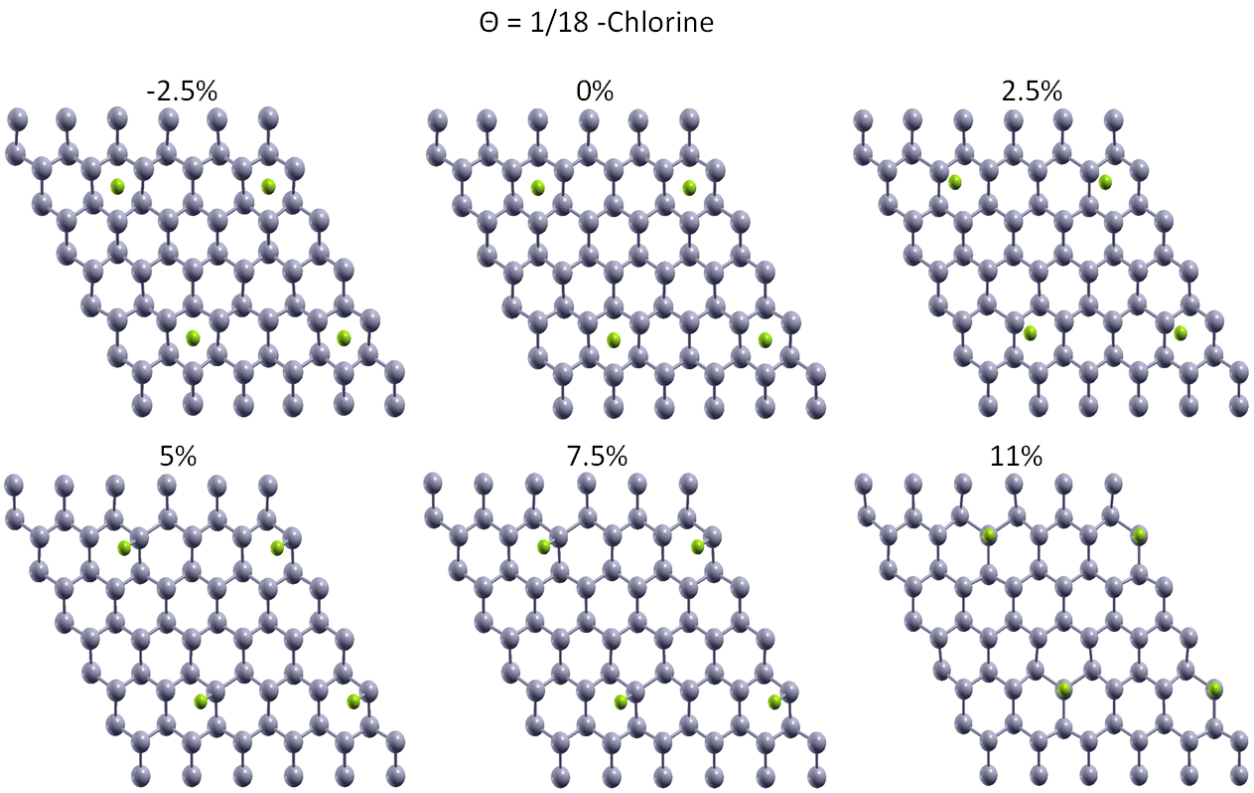

Fig. S8 Top view of the most stable site for the adsorption of Cl for Θ = 1/18. It is interesting to take note that at high bi-axial strain, there is a substantial change on the most stable site for Cl adsorption. In this case, the adsorption site change from the region around the hollow site to the top site.

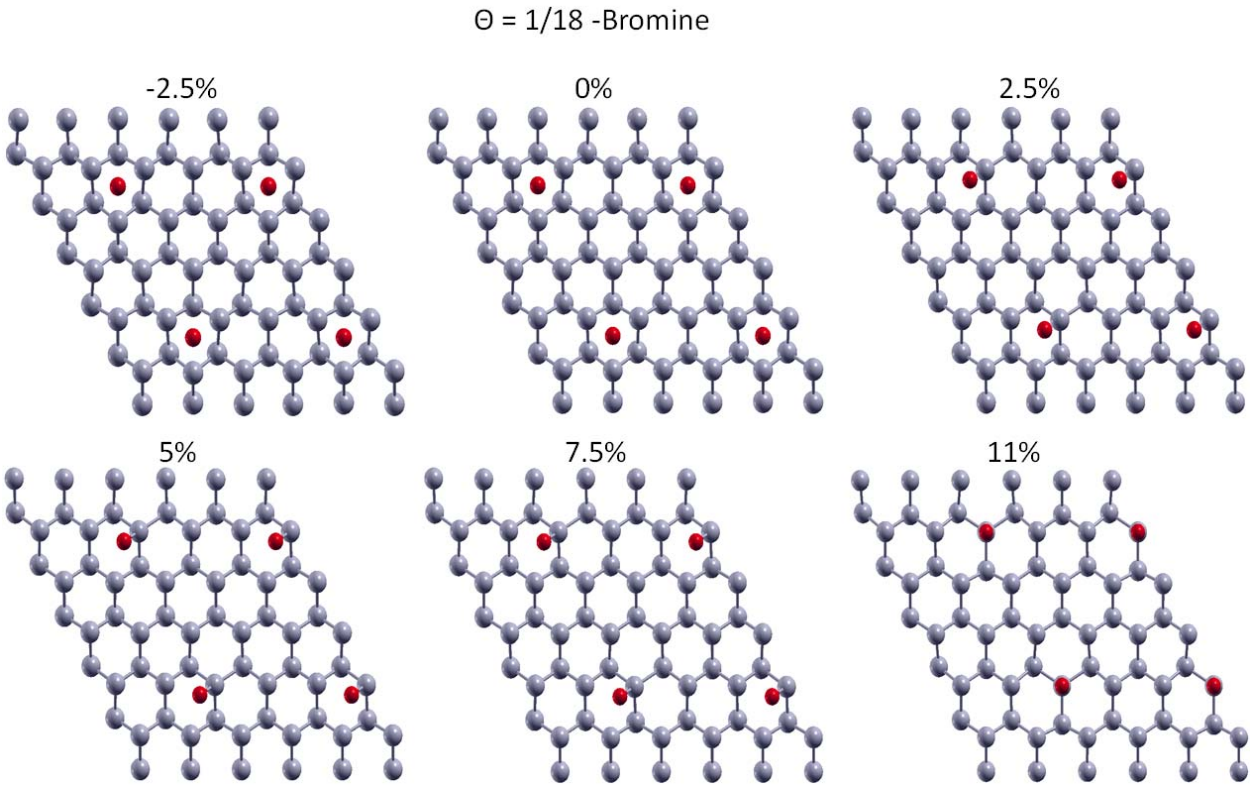

Fig. S9 Top view of the most stable site for the adsorption of Br for Θ = 1/18. It is interesting to take note that at high bi-axial strain, there is a substantial change on the most stable site for Br adsorption. In this case, the adsorption site change from the region around the hollow site to the top site.

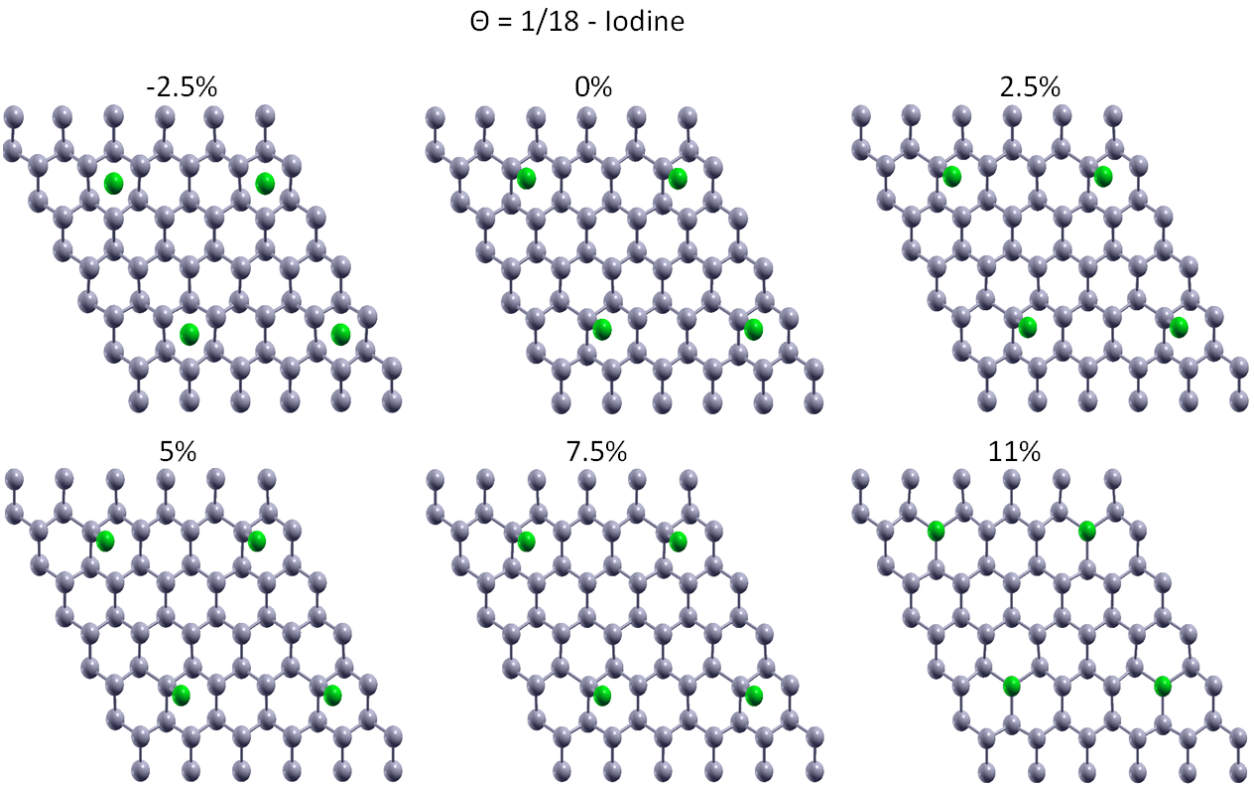

Fig. S10 Top view of the most stable site for the adsorption of I for Θ = 1/18. It is interesting to take note that at high bi-axial strain, there is a substantial change on the most stable site for I adsorption. In this case, the adsorption site change from the region around the hollow site to the top site.

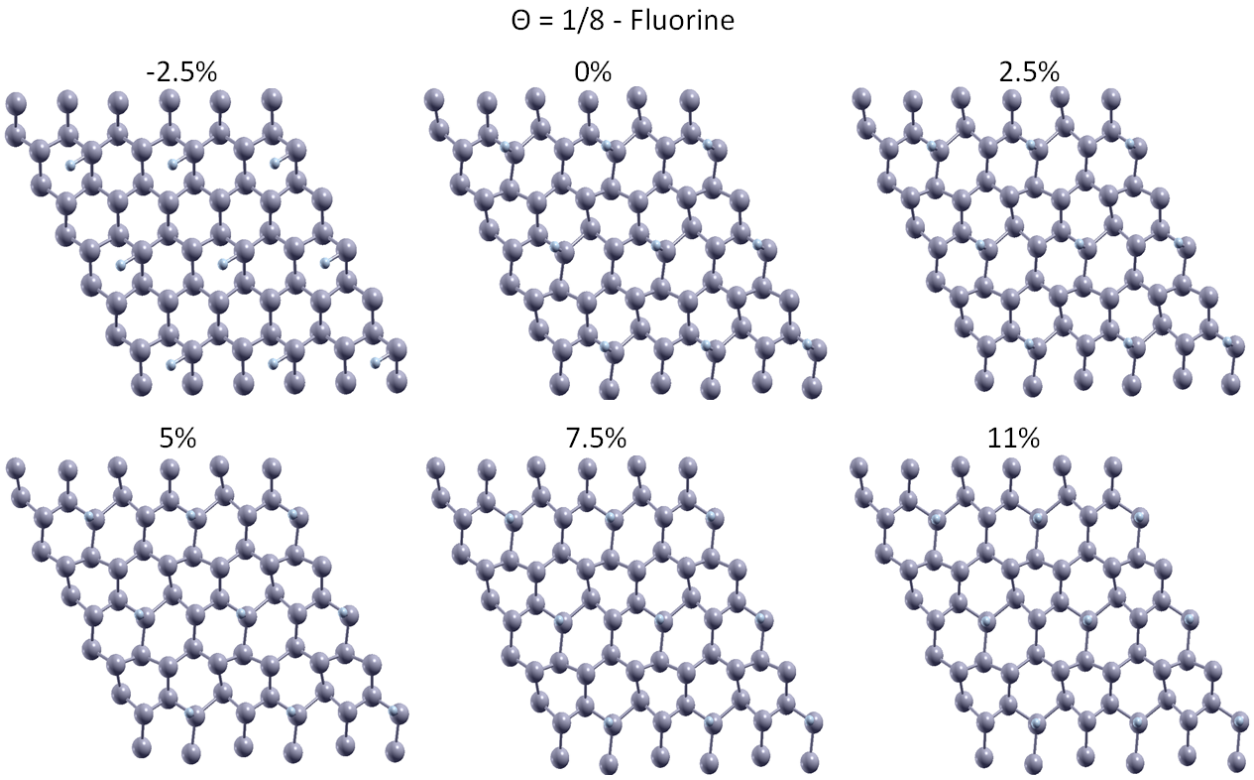

Fig S11 Top view of the most stable site for the adsorption of F for Θ = 1/8.

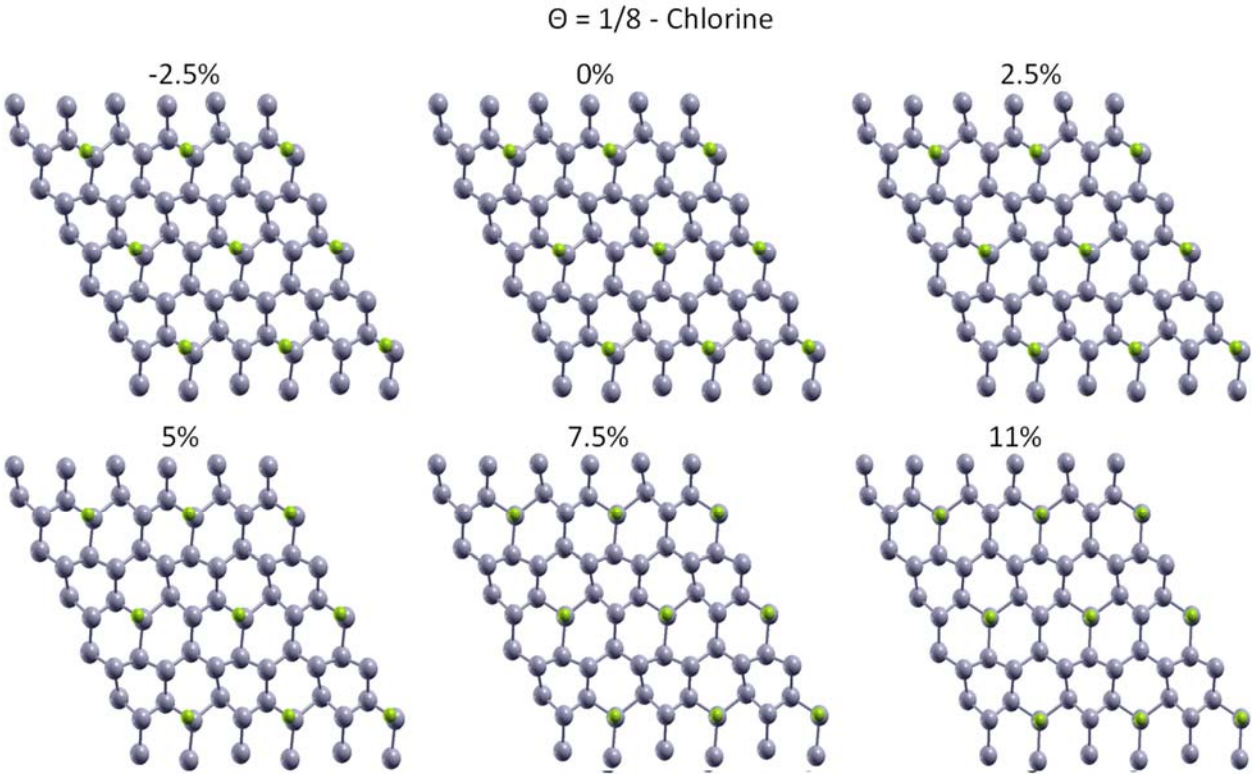

Fig S12 Top view of the most stable site for the adsorption of Cl for Θ = 1/8.

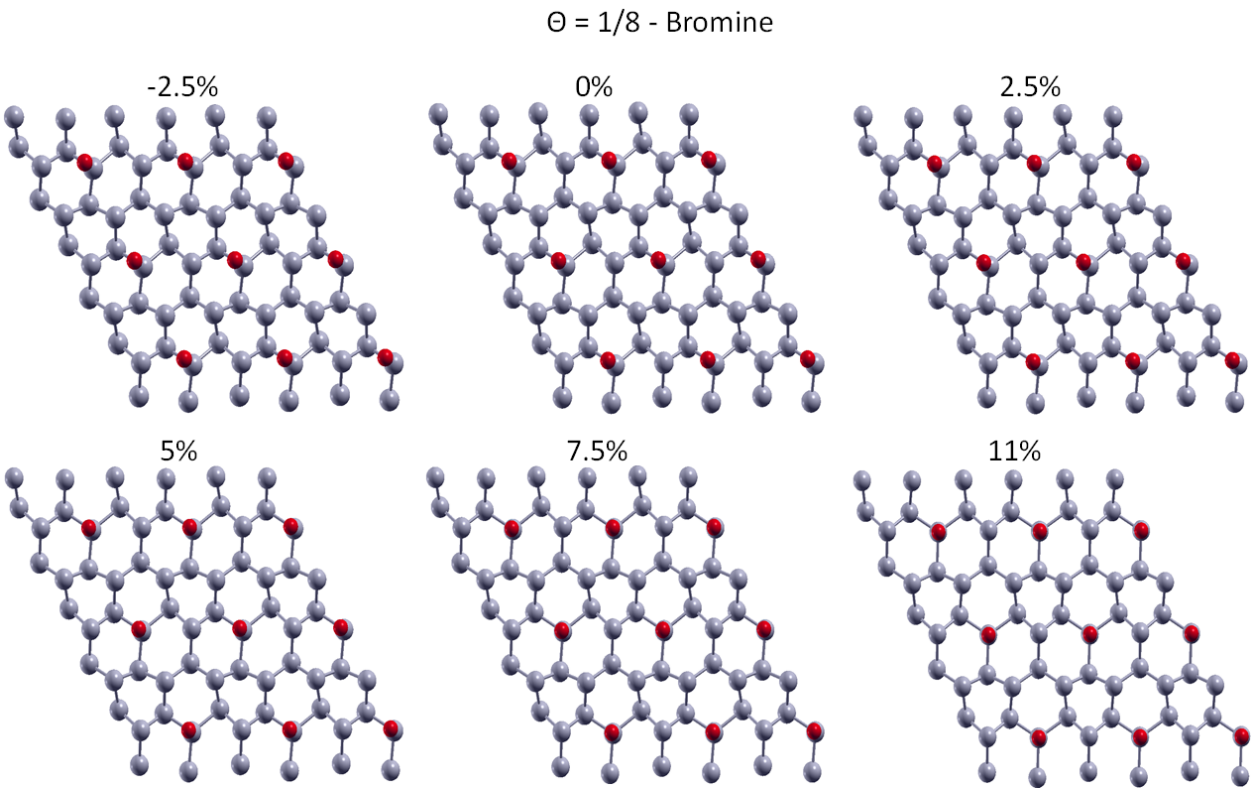

Fig S13 Top view of the most stable site for the adsorption of Br for Θ = 1/8.

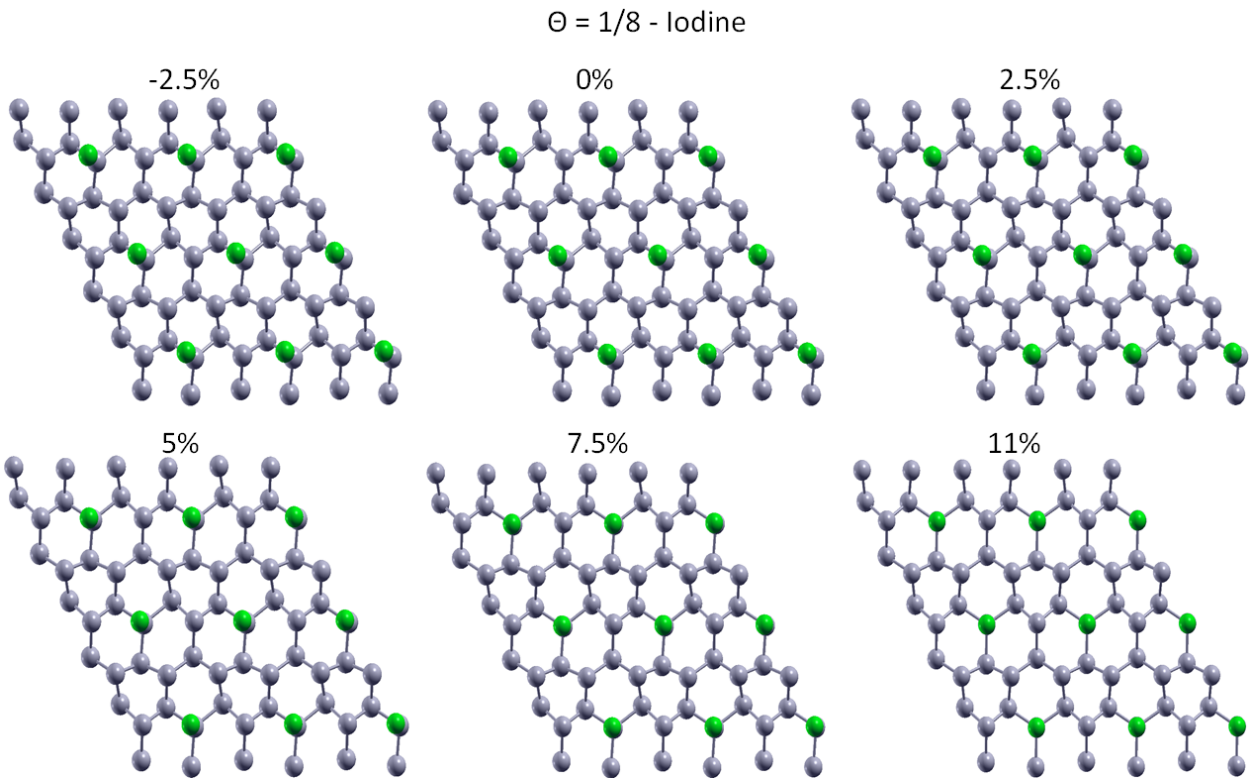

Fig S14 Top view of the most stable site for the adsorption of I for Θ = 1/8.