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

Supplementary material

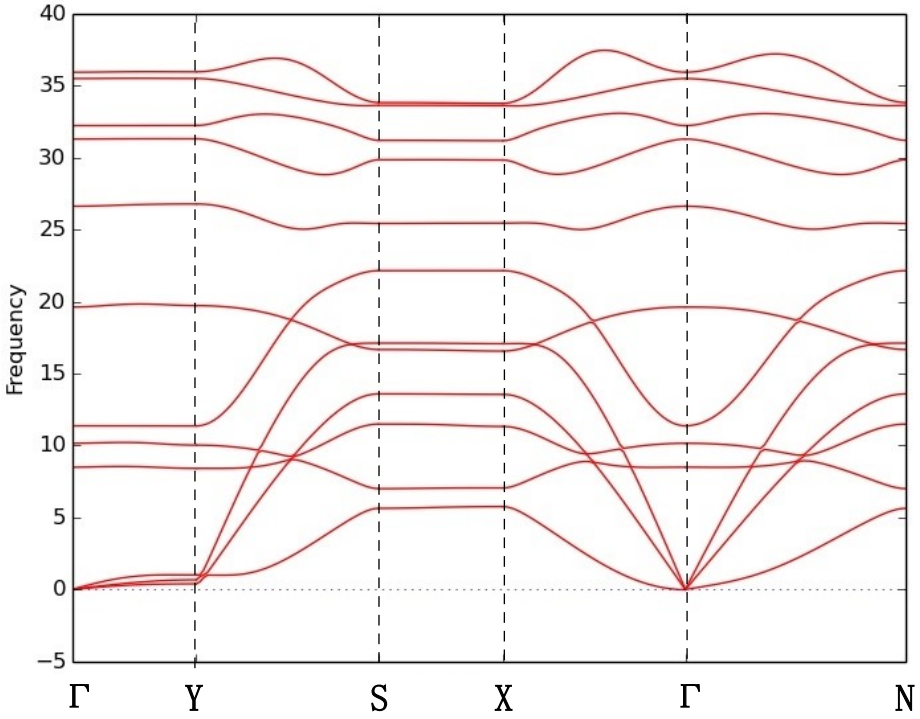


Fig.S1 Phonon dispersion of the BC_2P monolayer. The high symmetry points are Γ (0, 0, 0), Y(0, 0.5, 0), S/N(0.5, 0.5, 0) and X(0.5, 0, 0).

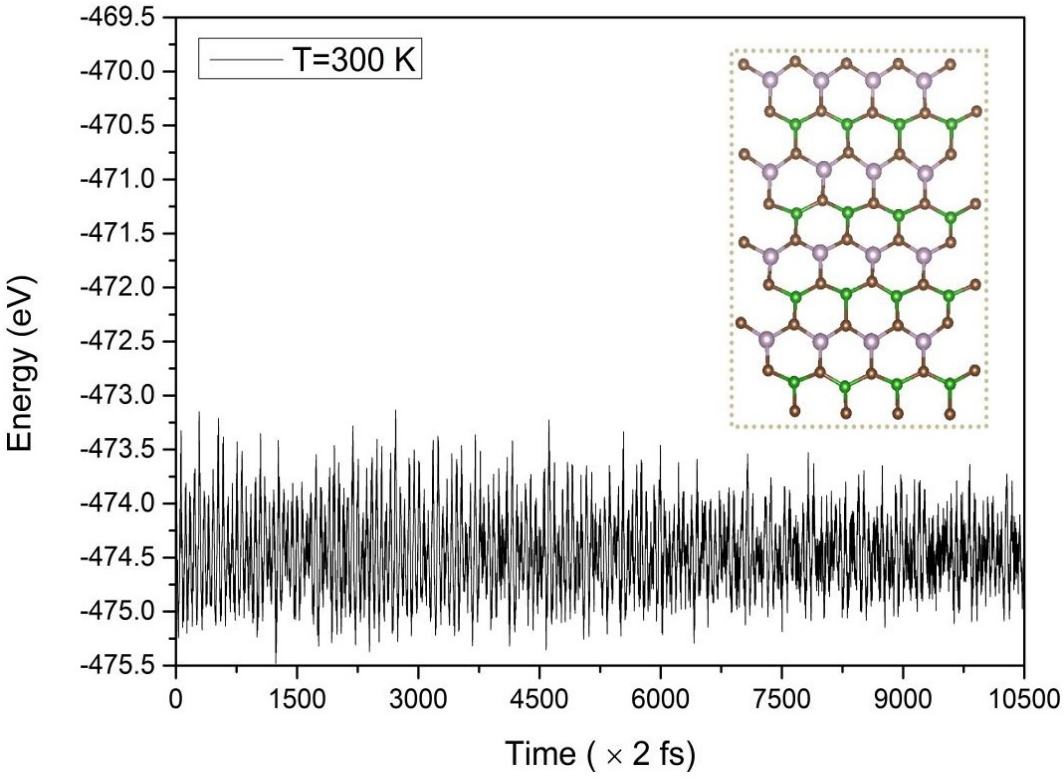
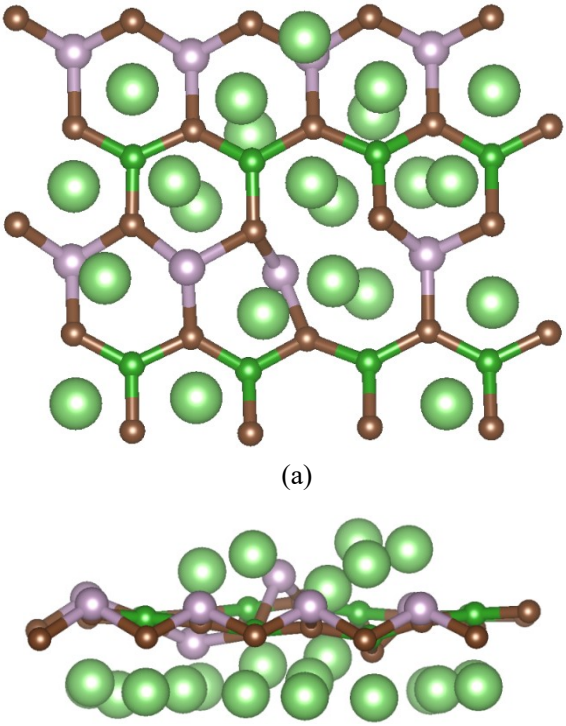


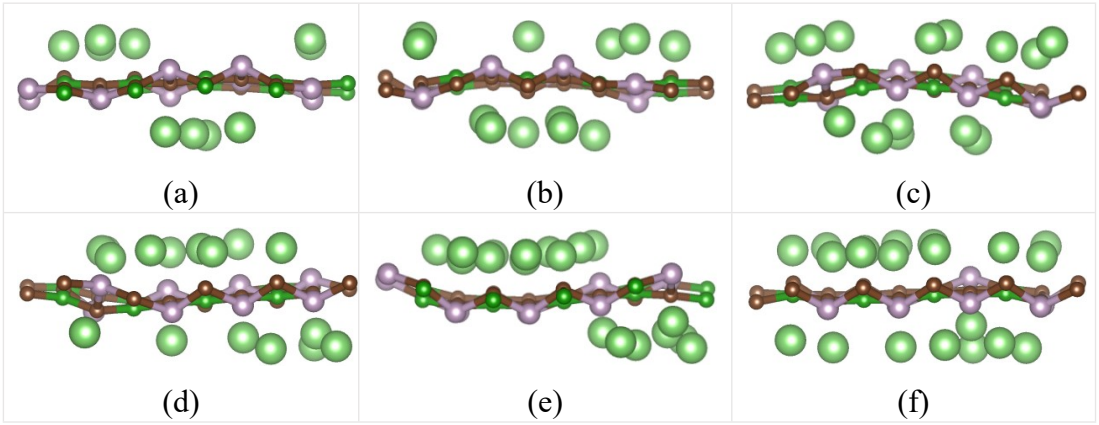
Fig.S2 Energy oscillations of the MD simulation at room temperature for the 3×3×1 supercell of BC_2P monolayer.



(a)

(b)

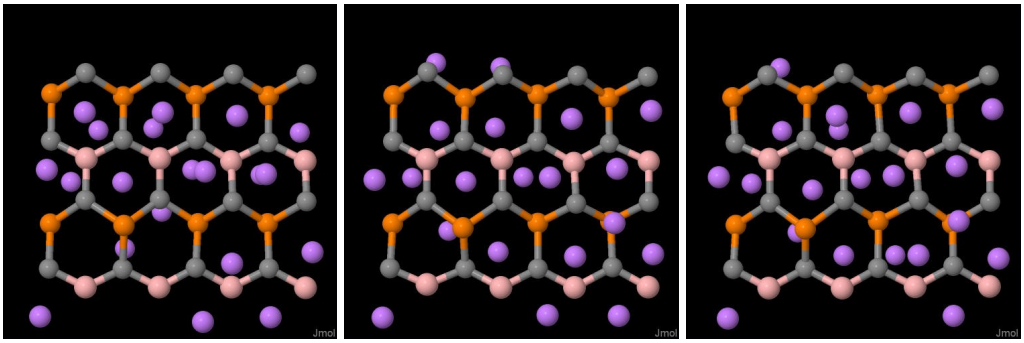
Fig.S3 Top and side views of optimized adsorption configuration with the number of adsorbed Li atoms as n=22.



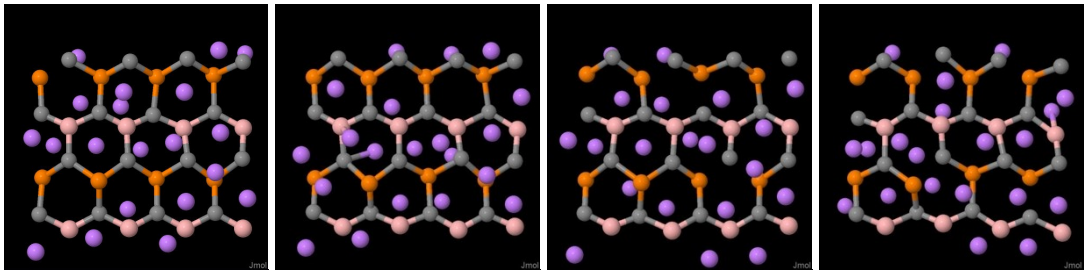
(a) (b) (c)

(d) (e) (f)

Fig.S4 The side views of optimized adsorption configuration for the six different Li concentrations with n=10, 12, 14, 16, 18, 20 (i.e. (a) $BC_2PLi_{1.25}$, (b) $BC_2PLi_{1.5}$, (c) $BC_2PLi_{1.75}$, (d) BC_2PLi_2 (e) $BC_2PLi_{2.25}$, (f) $BC_2PLi_{2.5}$).

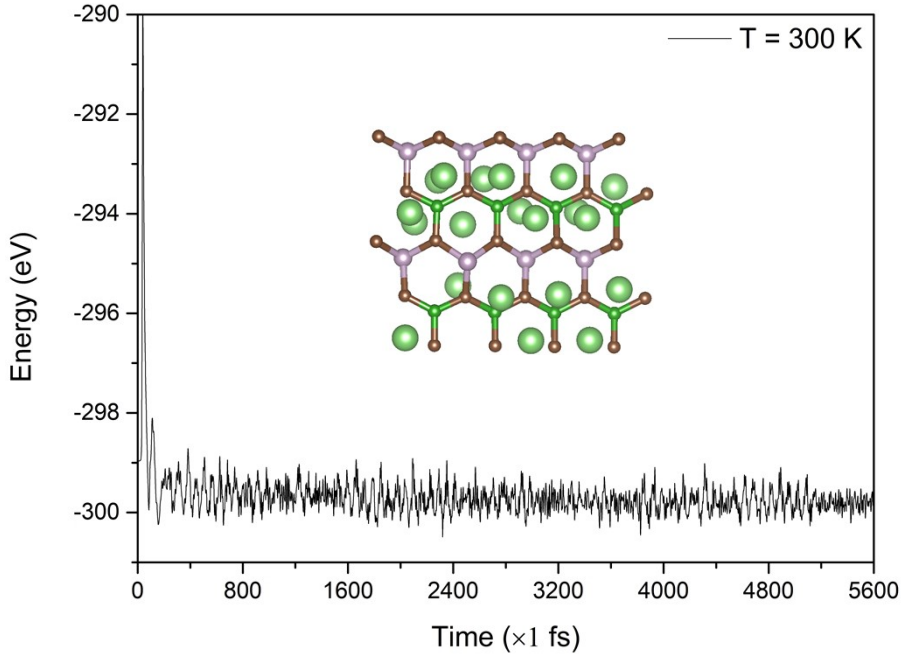


(1) T=100K (2) T=195K (3) T=310K



(4) T=585K (5) T=800K (6) T=1105K (7) T=1400K

(a)



(b)

Fig.S5 (a) Snapshots of the MD simulation for the $Li_{2.5}BC_2P$ supercell with the temperature from 100K to 1400K. (b) Energy oscillations of the equilibrium MD simulation at room temperature 300 K for the $Li_{2.5}BC_2P$ supercell.

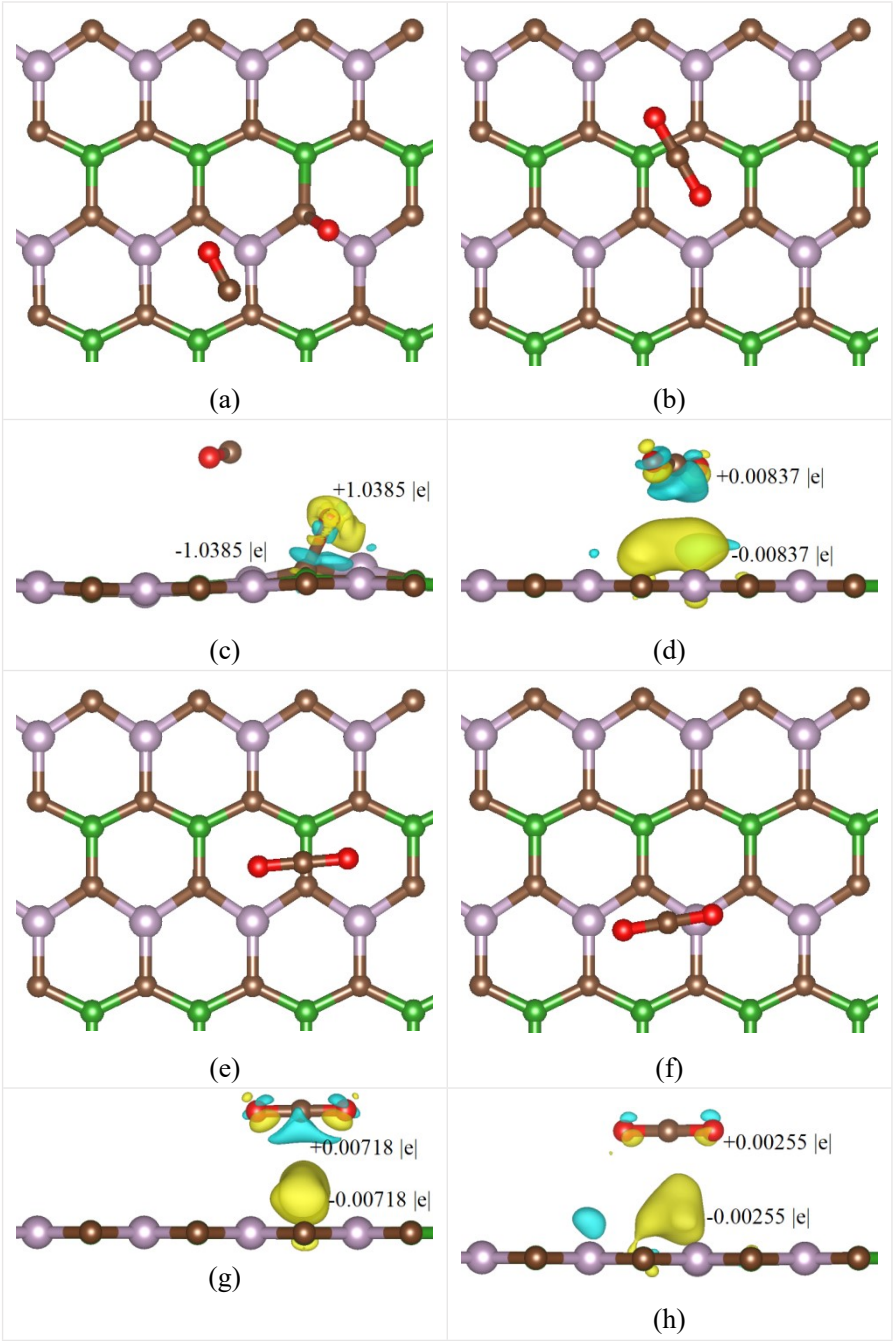


Fig.S6 (a), (c) Top and side views of the top sites of C atoms on the supercell of BC_2P monolayer with the ISO as 0.015 $e^-/Bohr^3$. (b), (d), (e), (g) and (f), (h) Top and side views of two B-C bond sites and the B-C bond site on the BC_2P supercell, which including the CDD and the ISO 0.0003 $e^-/Bohr^3$.

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