

Supplementary data for

Elimination of interlayer Schottky barrier in borophene/C₄N₄ vdW heterojunction *via* Li-ions adsorption for tunneling photodiode

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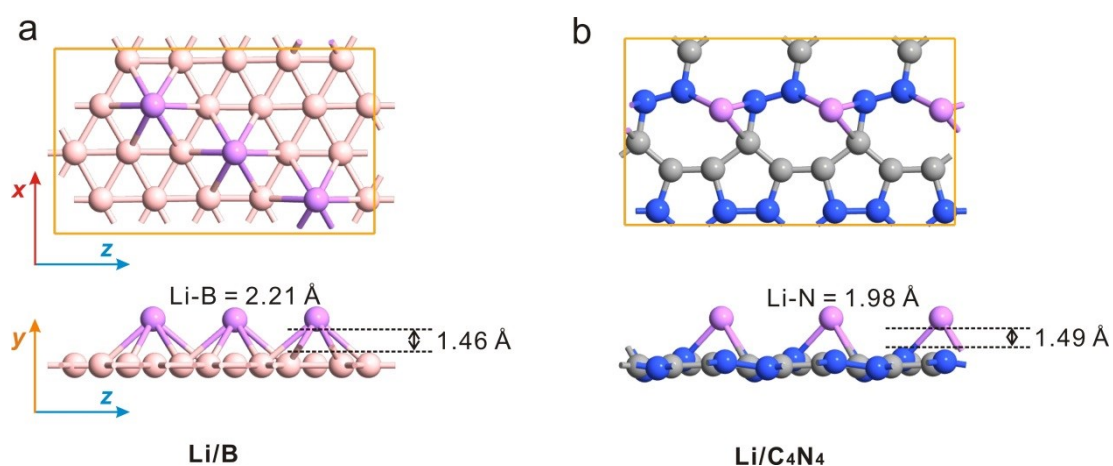


Fig. S1 Top and side views of (a) Li-ions-adsorbed borophene (Li/B) and (b) Li-ions-adsorbed C₄N₄ (Li/C₄N₄) monolayers, respectively.

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Table S1 The lattice constants along x (a) and z (c) directions, binding energy (E_b), the interlayer distance (d_y) in Li/B and Li/C₄N₄ monolayers, respectively.

	$a/\text{\AA}$	$c/\text{\AA}$	$E_b/\text{eV/atom}$	$d_y/\text{\AA}$	$L_{\text{Li-X}}/\text{\AA}$	$\Delta\Phi/\text{eV}$
Li/B	5.86	10.13	-0.46	1.46	2.21 (Li-B)	-3.44
Li/C ₄ N ₄	6.08	10.77	-0.23	1.49	1.98 (Li-N)	-4.55

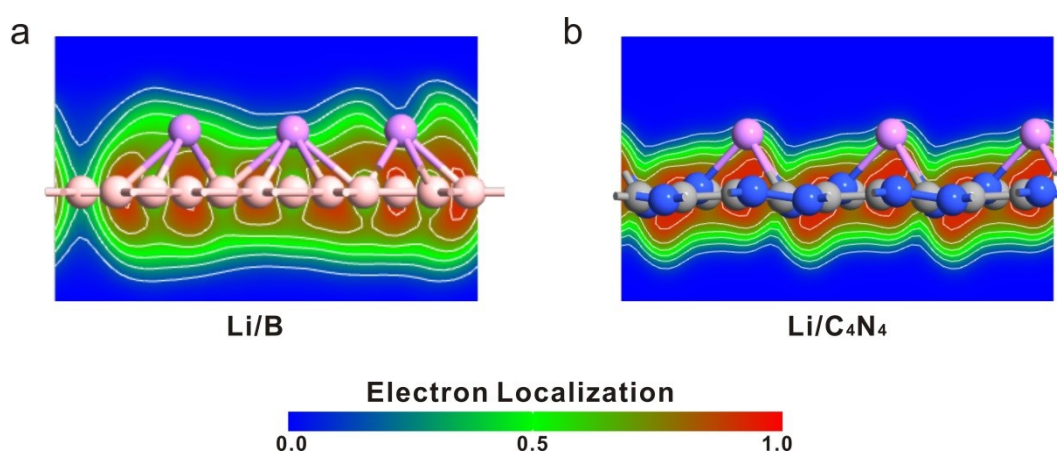


Fig. S2 Side views of ELF maps for (a) Li/B and (b) Li/C₄N₄ monolayers, respectively.