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

Oxygen-substituted borophene as a potential anode material for Li/Na-ion batteries: A first principles study

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Supplementary information:

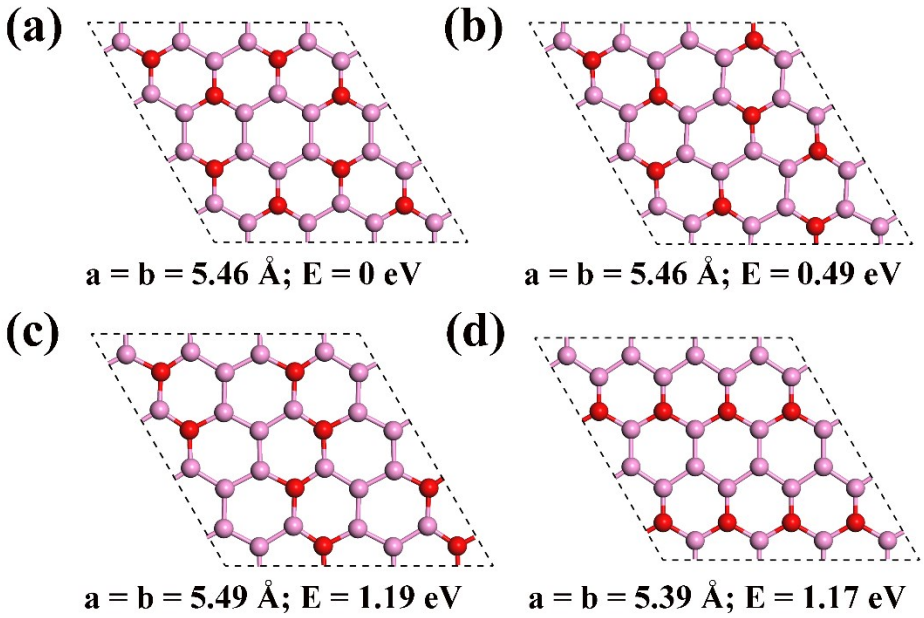

Figure S1 Optimized low-energy geometries of HBS oxides. The corresponding lattice constants and energies are labeled down below.

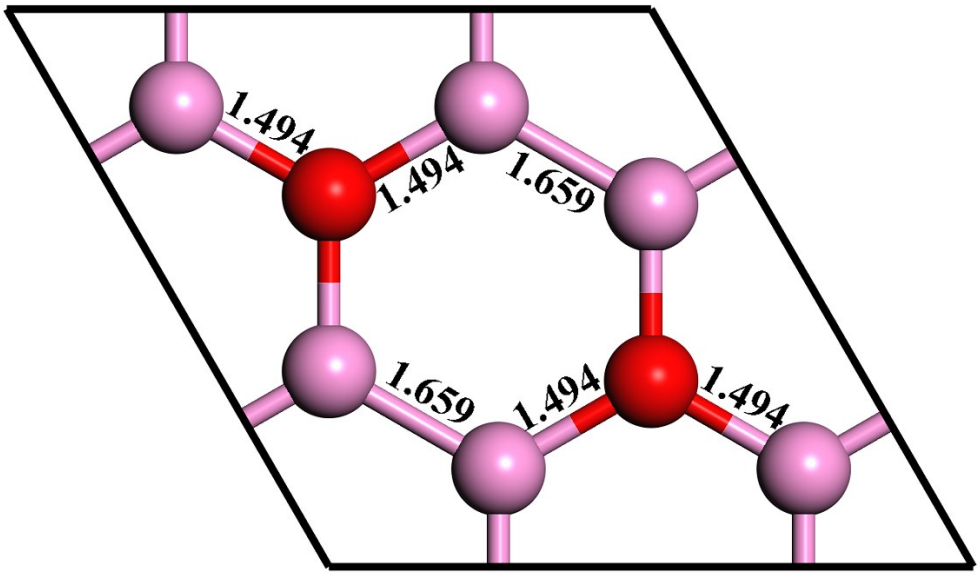

Figure S2 Optimized unit structure of *h*-B_3O monolayer, bond lengths are in angstroms (Å).

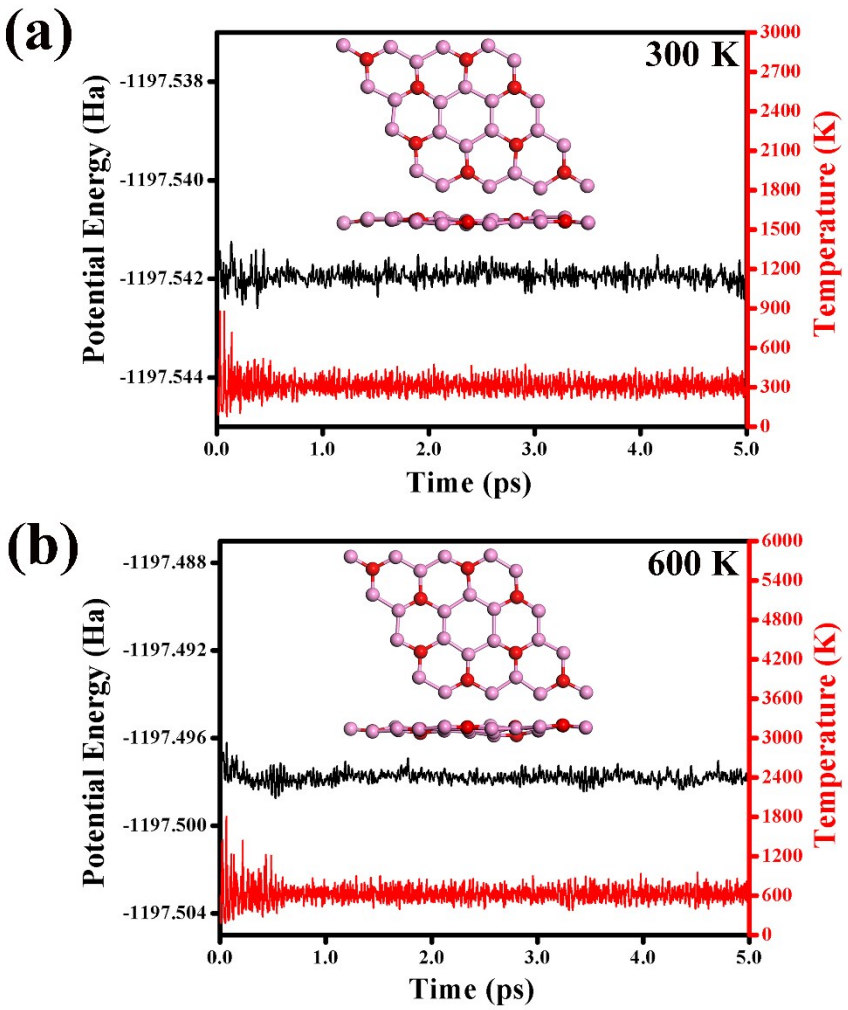

Figure S3 Variation of the potential energies and the temperatures of *h*-B_3O monolayer in molecular dynamics (MD) simulations at (a) 300 K and (b) 600 K, the corresponding snapshots of the final frame of *h*-B_3O monolayer after lasting for 5.0 ps.

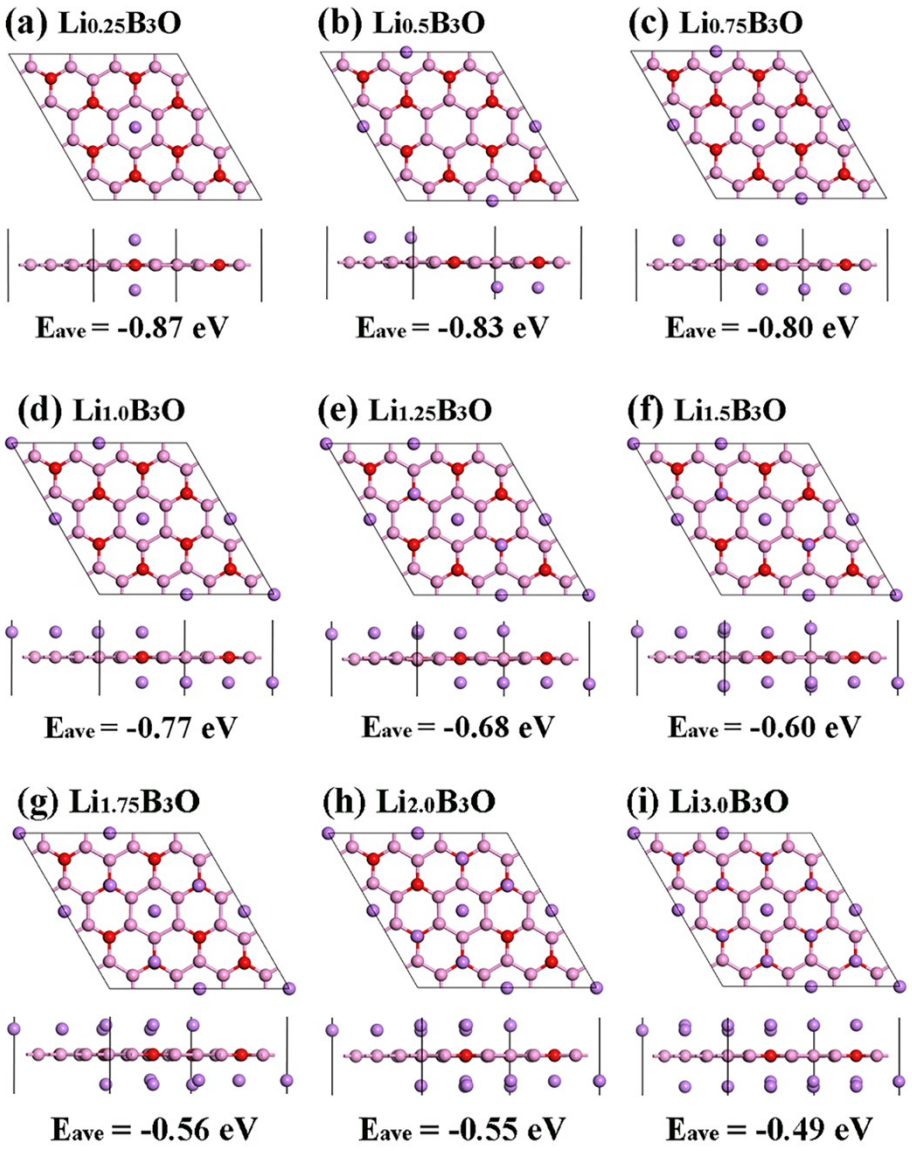

Figure S4 Top and side views of the optimized structures of (a) $Li_{0.25}B_3O$; (b) $Li_{0.5}B_3O$; (c) $Li_{0.75}B_3O$; (d) $Li_{1.0}B_3O$; (e) $Li_{1.25}B_3O$; (f) $Li_{1.5}B_3O$; (g) $Li_{1.75}B_3O$; (h) $Li_{2.0}B_3O$ and (i) $Li_{3.0}B_3O$ with Li atoms adsorbed on the surface of *h*-B_3O monolayer. The B, O and Li atoms are denoted by pink, red and purple balls, respectively.

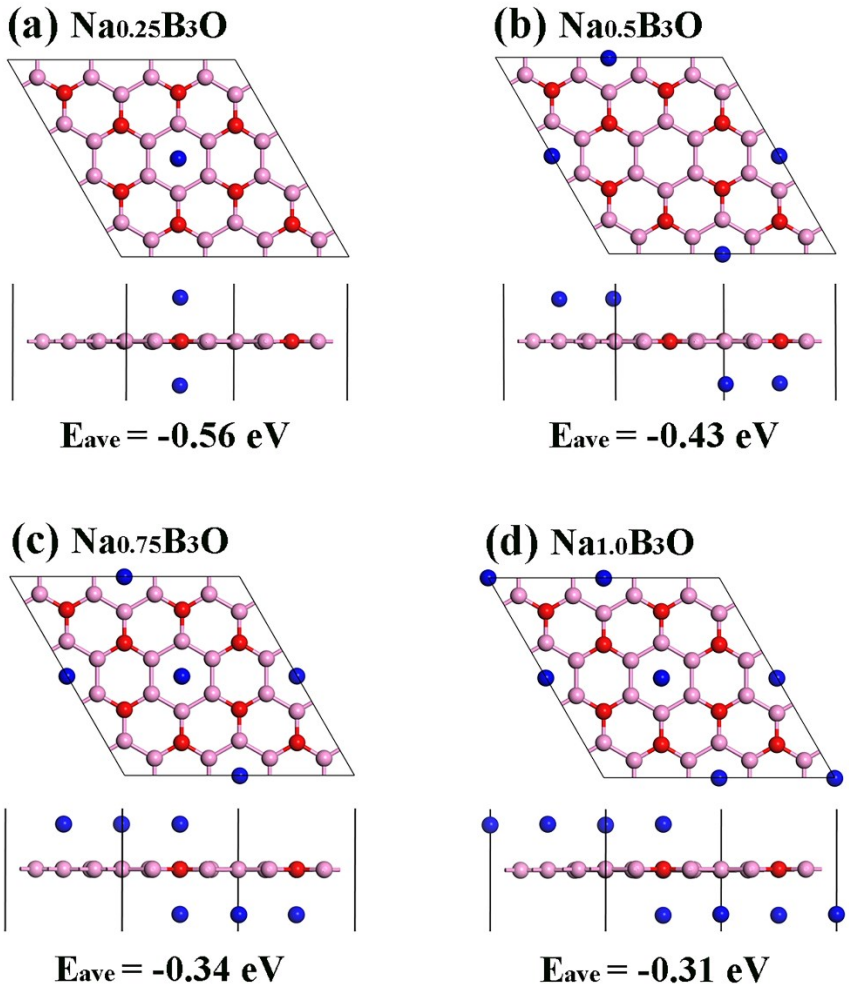

Figure S5 Top and side views of the optimized structures of (a) $Na_{0.25}B_3O$; (b) $Na_{0.5}B_3O$; (c) $Na_{0.75}B_3O$ and (d) $Na_{1.0}B_3O$ with Na atoms adsorbed on the surface of *h*-B_3O monolayer. The B, O and Na atoms are denoted by pink, red and blue balls, respectively.

Table S1 The adsorption energies, initial sites, final sites and adsorption heights for Li/Na atom adsorbed on *h*-B_3O monolayer surface.

Metal atoms	Initial sites	Final sites	Adsorption energies (eV)	Adsorption heights (Å)
Li	**H1**	**H1**	**-2.33**	**1.818**
	H2	**H2**	**-1.86**	**1.712**
	T1	**H1**	**-2.33**	**1.809**
	T2	**H2**	**-1.86**	**1.701**
	B1	**H1**	**-2.33**	**1.792**
	B2	**H2**	**-1.86**	**1.717**
Na	**H1**	**H1**	**-1.70**	**2.311**
	H2	**H2**	**-1.33**	**2.243**
	T1	**H1**	**-1.70**	**2.293**
	T2	**T2**	**-1.27**	**2.077**
	B1	**H2**	**-1.33**	**2.250**
	B2	**T2**	**-1.27**	**2.100**