Bi-Modified V_2C MXene Monolayer Film as Anode for Alkali Metal Ion (Li/Na) Batteries: A First-Principles Study

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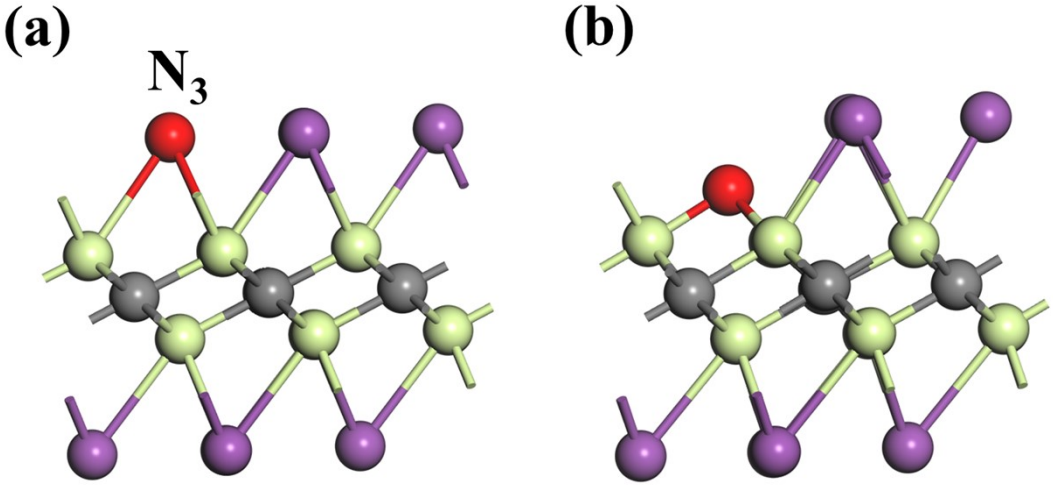

Fig.S1 Side view of O atoms doped at N_3 site of V_2CBi_2 before(a) and after optimization(b).

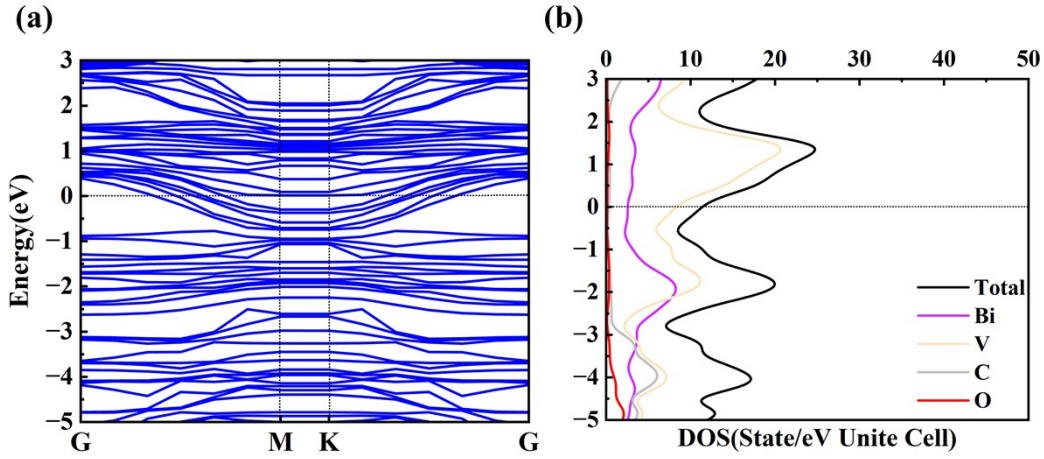

Fig.S2 Band structure (a) and density of states (b) of O-doped V_2CBi_2

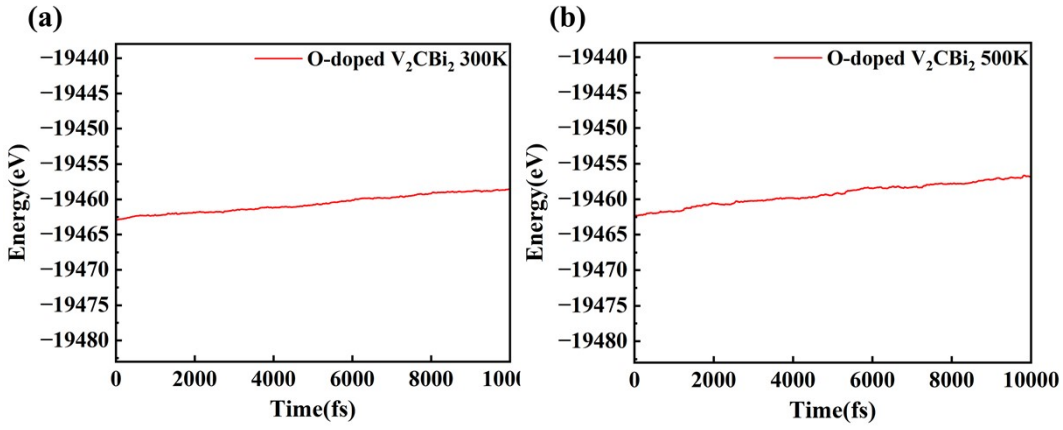

Fig.S3 Evolution of free energy of O-doped V_2CBi_2 in AIMD caculations at 300 K (a) and at 500 K (b) during the time scale of 1 fs.

Table S1. Elastic constants (N/m) of V_2CBi_2 monolayer.

	C_{11} (N/m)	C_{22} (N/m)	C_{12} (N/m)	C_{66} (N/m)
V_2CBi_2	189.22	181.788	80.408	52.277

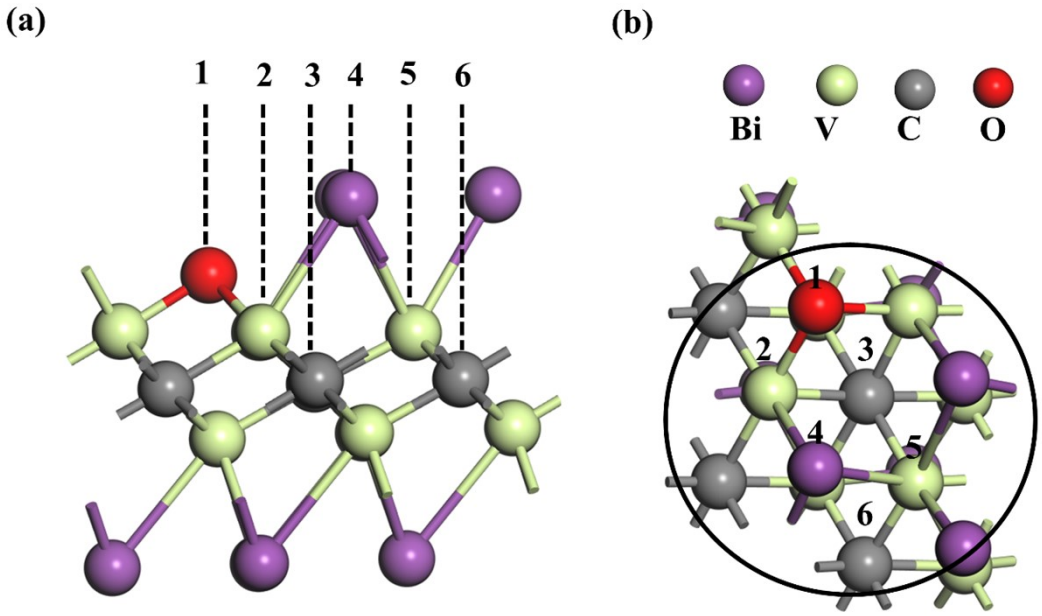

Fig.S4 Side view (a) and top view (b) of the six possible adsorption sites at O-doped V_2CBi_2 monolayer.

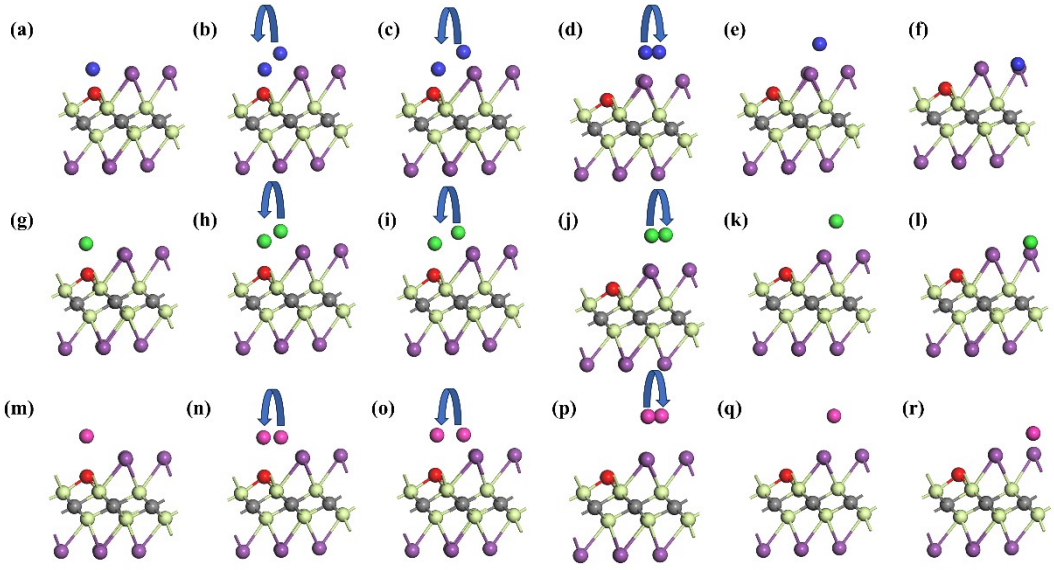

Fig.S5 Side view of Li(a–f), Na(g–l) and K(m–r) atoms adsorbed at six different sites (1, 2, 3, 4, 5, 6) of O-doped V_2CBi_2 respectively after optimization.

Table S2. The adsorption energies of Li/Na/K at different sites on O-doped V_2CBi_2.

Sites	**Adsorbate & Eads(eV)**		
	Li	**Na**	**K**
1	−3.52	−2.92	−2.58
2	−3.52	−2.92	−2.58
3	−3.52	−2.92	−2.58

4	−2.13	−1.55	−1.54
5	−2.13	−1.55	−1.54
6	−3.12	−2.50	−2.37

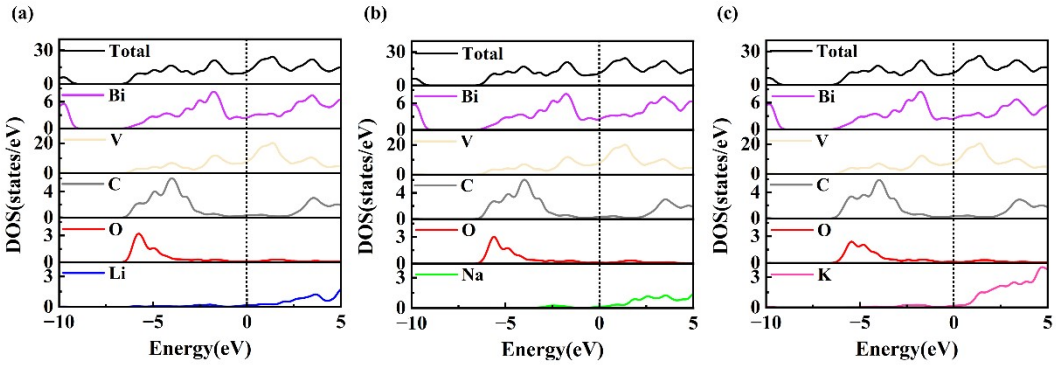

Fig.S6. Total and projected density of states for Li/Na/K adsorbed on O-doped V_2CBi_2.

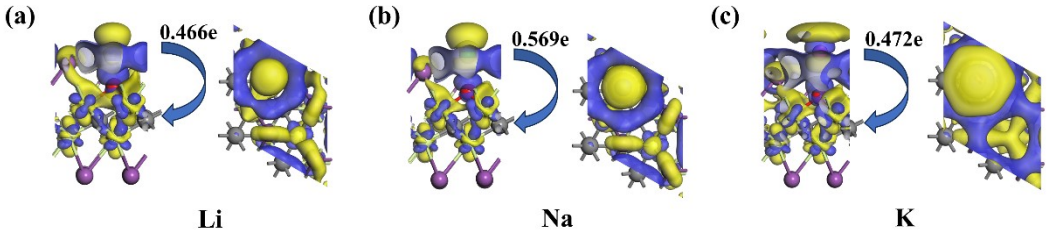

Fig.S7. The charge density difference (CDD) and Mulliken charge for Li, Na, K, ions adsorbed at 1 site on the O-doped V_2CBi_2 (a–c).

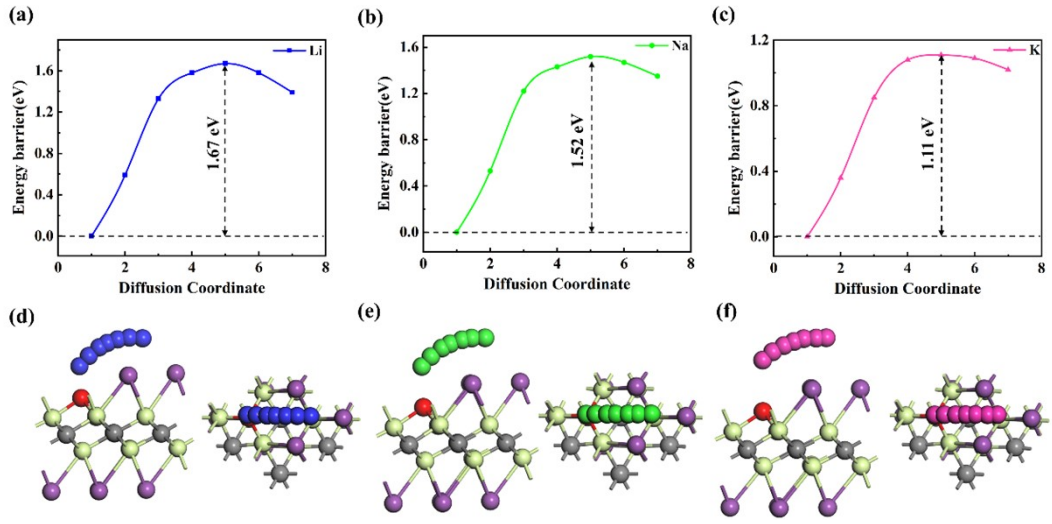

Fig.S8. The diffusion barriers (a–c) and diffusion path (d–f) for Li/Na/K atoms on O-doped V_2CBi_2.