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

Supporting Information for

Prediction of Two-Dimensional PC_6 as a Promising Anode Material for Potassium-Ion Battery

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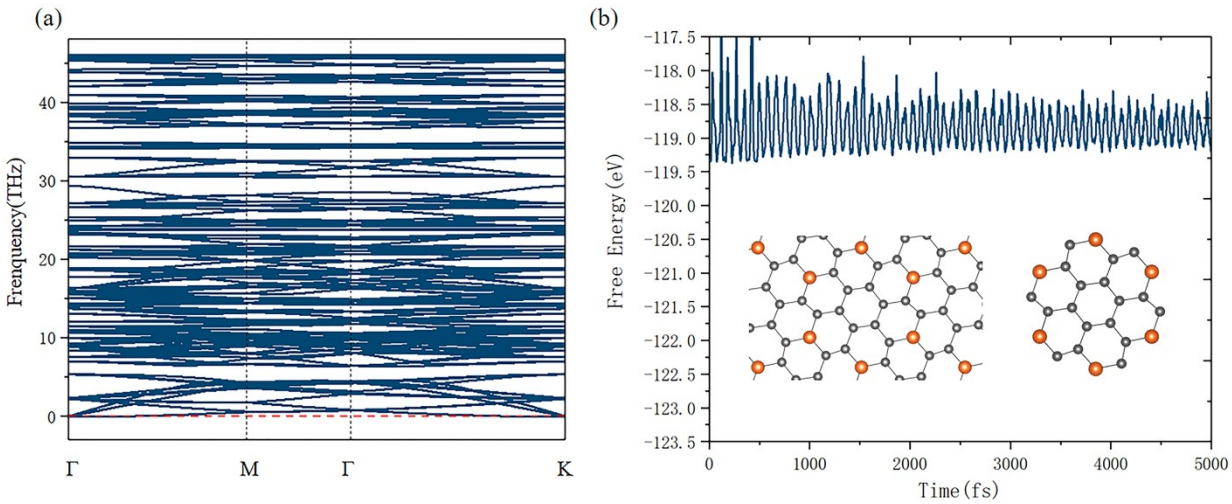

Fig S1. (a)Calculated phonon band structure of the PC_6 monolayer. (b)AIMD simulation over 5ps at 300K.

Fig. S1 (a) Phonon spectrum of PC_6 monolayer. (b) Fluctuations of total energy with time obtained from MD simulation of PC_6 monolayer at 300 K. Insert in (b) is the snapshot of PC_6 monolayer at the end of MD simulation.

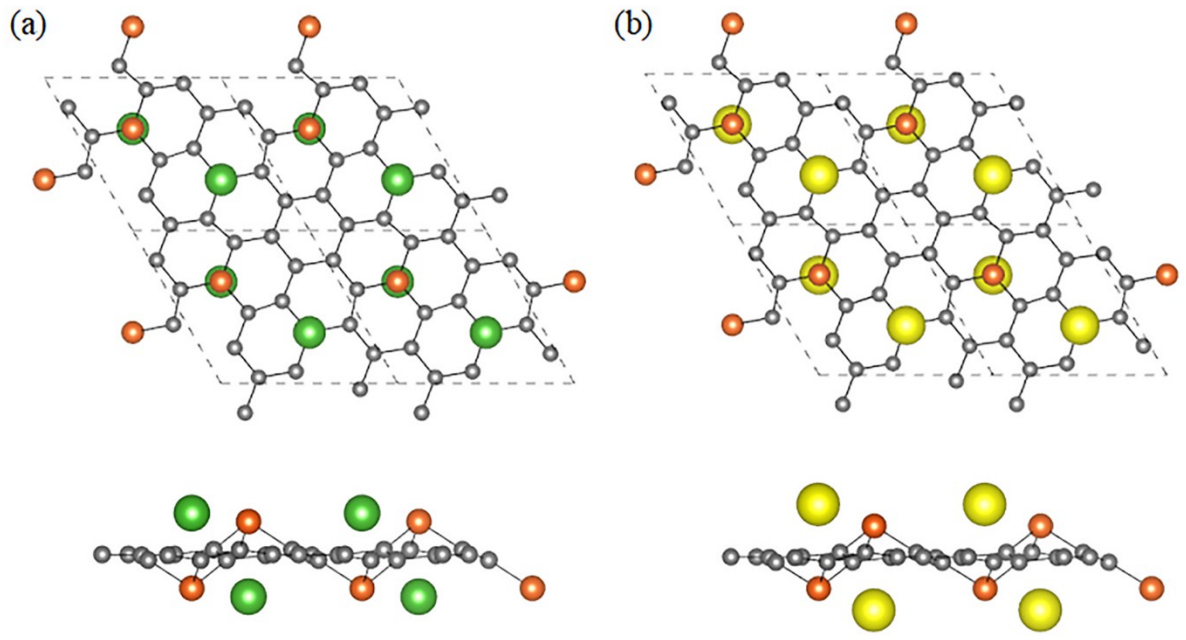

Fig. S2 Adsorption structure of PC_6Li_1 (a) and PC_6Na_1(b). Green balls indicate Li atoms and yellow balls indicate Na atoms.

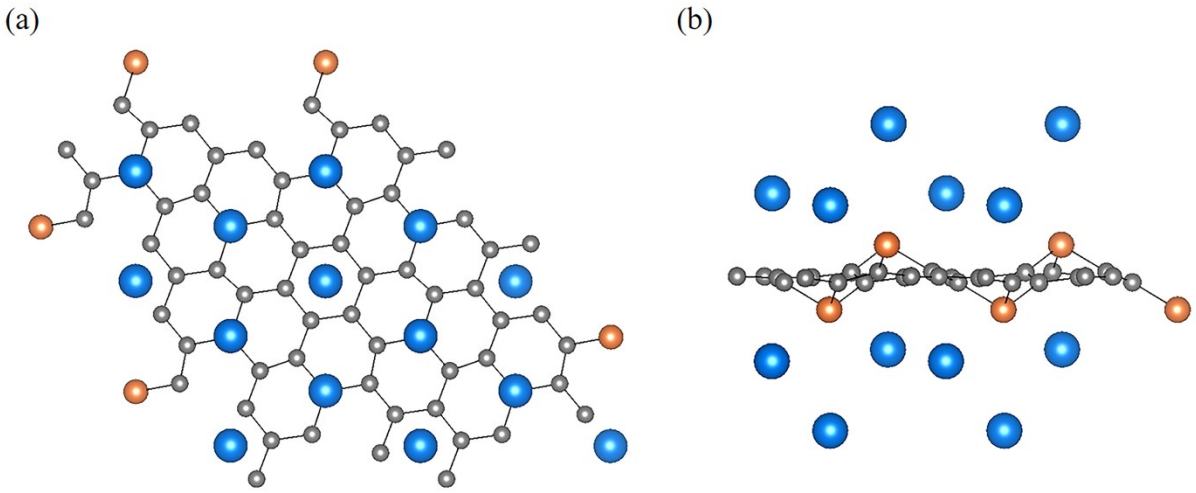

Fig. S3 Crystal structure of PC_6 monolayer with full K ions adsorption after AIMD simulations at 300 K for 3ps from top (a) and side (b) views. Blue balls indicate K atoms.

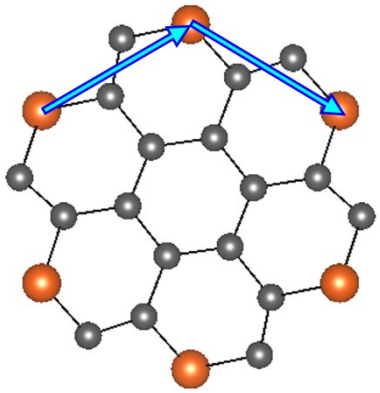

Fig. S4 Schematic illustrations for the migration path Ⅲ of K diffusion on the surface of PC_6 monolayer. We investigate the diffusion path along the zigzag direction which is shown in **Fig. S4**. The corresponding diffusion barrier is estimated to be 0.97 eV, which is much higher than diffusion barriers along path Ⅰ (0.27 eV) and path Ⅱ (0.26 eV) shown in **Fig 3(a)**, indicating this path is not favorable.

Table S1. Adsorption energy (E_{ad}), adsorption height (h), and Bader charge analysis (E_b) of PC_6 monolayer with the adsorption of single K atom in different configurations.

Site	E_{ad} (eV)	h (Å)	E_b (e)
S1	-1.34	1.20	0.891
S4	-1.12	1.55	0.899
S6	-0.44	2.96	0.860
S5		S4	
S2/S3/S7/S8		S1	

Table S2. Adsorption Energy (E_{ad}) and adsorption Height (h) of Li-Adsorbed PC_6 and Na-adsorbed PC_6 in different adsorption sites.

Site	E_{ad} (eV)	h (Å)	E_{ad} (eV)	h (Å)
	Li-adsorption		Na-adsorption	
S1	-0.63	0.34	-0.74	0.75
S4	-0.44	0.72	-0.46	1.15
S6	0.37	2.40	0.13	2.74
S5	S4		S4	
S2/S3/S7/S8	S1		S1	

Table S3. Adsorption energy (E_{ad}) and adsorption height (h) of two-layer K-adsorbed PC_6 with the adsorption of single K atom for the third layer in different sites.

Site	E_{ad} (eV)	h (Å)
S1	0.89	3.42
S4	0.51	3.89
S6	-0.45	2.03