

Supporting Information

Two-dimensional monolayer C₅₋₁₀₋₁₆: a metallic carbon allotrope as an anode material of high-performance sodium/potassium-ion batteries

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1. Phonon spectra of $C_{5-10-16}$ monolayer

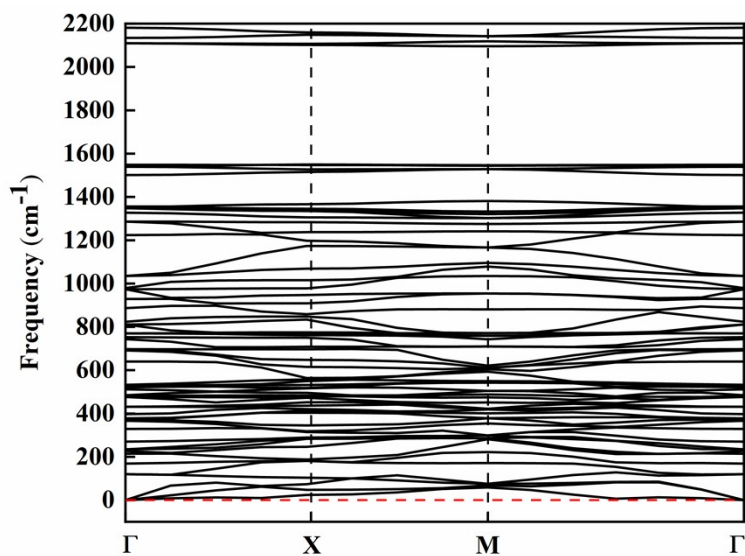


Fig. S1. Phonon spectra of $C_{5-10-16}$ monolayer.

2. The 17 possible adsorption sites on monolayer $C_{5-10-16}$

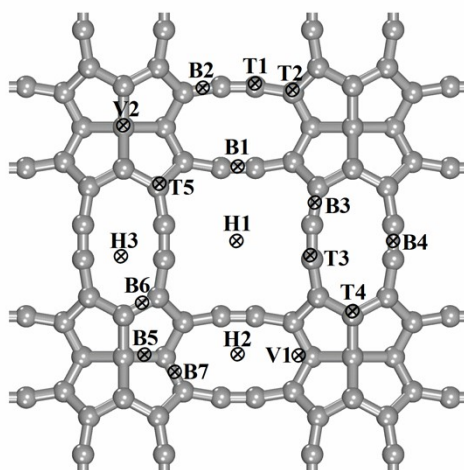


Fig. S2. 17 Possible adsorption sites.

3. Initial and final adsorption sites on monolayer C₅₋₁₀₋₁₆

Table S1 Initial and final adsorption sites on C₅₋₁₀₋₁₆.

	Initial site of Na(K)	Final site of Na(K)
	H1	H1(H1)
	H2	H2(H2)
	V1	V1(H2)
	H3	H3(H3)
	V2	V2(V2)
	B1	H2(H2)
	T1	H2(H2)
	B2	H2(H2)
Possible adsorption sites	T2	V1(H2)
	B7	V1(H2)
	B3	H3(H3)
	T3	H3(H3)
	B4	H3(H3)
	T5	H3(H3)
	T4	V2(V2)
	B5	V2(V2)
	B6	V2(V2)

4. The $E_{\text{diff-ads}}$ of Na and K atoms on the $C_{5-10-16}$ monolayer

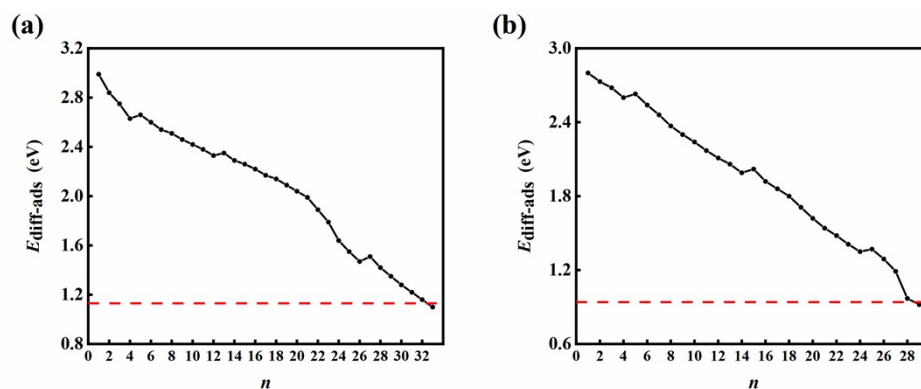


Fig. S3. $E_{\text{diff-ads}}$ of (a) Na and (b) K atoms on the $C_{5-10-16}$ monolayer. The red dashed line represents the cohesive energy of bulk Na/K (1.13 eV/0.94 eV).

5. The average interlayer distance (D) of $C_{5-10-16}$ bilayer with adsorbed Na

Table S2 The average interlayer distance (D) of $C_{5-10-16}$ bilayer with adsorbed Na.

	site	D
Outside surface of the $C_{5-10-16}$ bilayer	H1	3.45 Å
	H2	3.53 Å
	V1	3.54 Å
	H3	3.52 Å
	V2	3.55 Å
Interlayer of the $C_{5-10-16}$ bilayer	H1	3.46 Å
	H2	3.76 Å
	H3	3.76 Å

6. The average interlayer distance (D) of $C_{5-10-16}$ bilayer with adsorbed K

Table S3 The average interlayer distance (D) of $C_{5-10-16}$ bilayer with adsorbed K.

	site	D
Outside surface of the $C_{5-10-16}$ bilayer	H1	3.54 Å
	H2	3.54 Å
	H3	3.53 Å
	V2	3.55 Å
Interlayer of the $C_{5-10-16}$ bilayer	H2	4.09 Å
	H3	4.09 Å
	V2	4.15 Å