Supporting Information

Two-dimensional azulenoid kekulenes based metallic allotropes for energy storage applications

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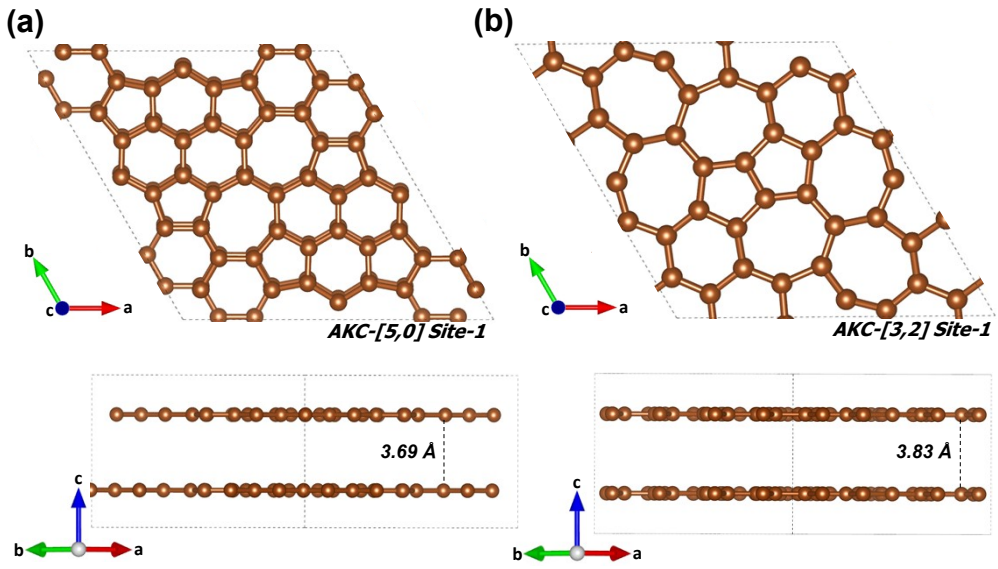

Figure. S1 Top and side view of fully relaxed geometry of AA-stacking for metallic (a) AKC-5,0 and (b) AKC-3,2 carbon allotropes.

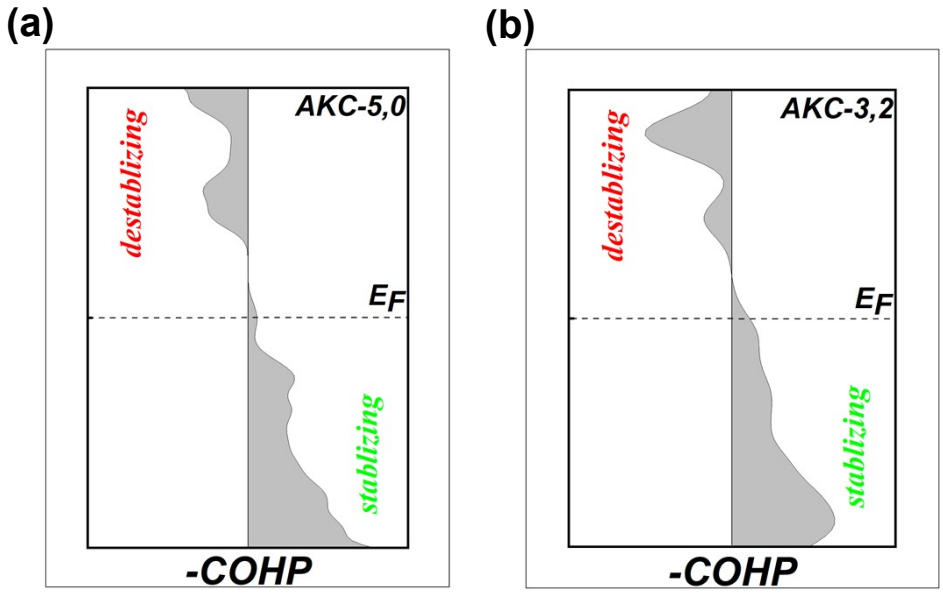

Figure. S2 The crystal orbital Hamilton population (COHP) analysis for metallic (a) AKC-5,0 and (b) AKC-3,2 carbon allotropes.

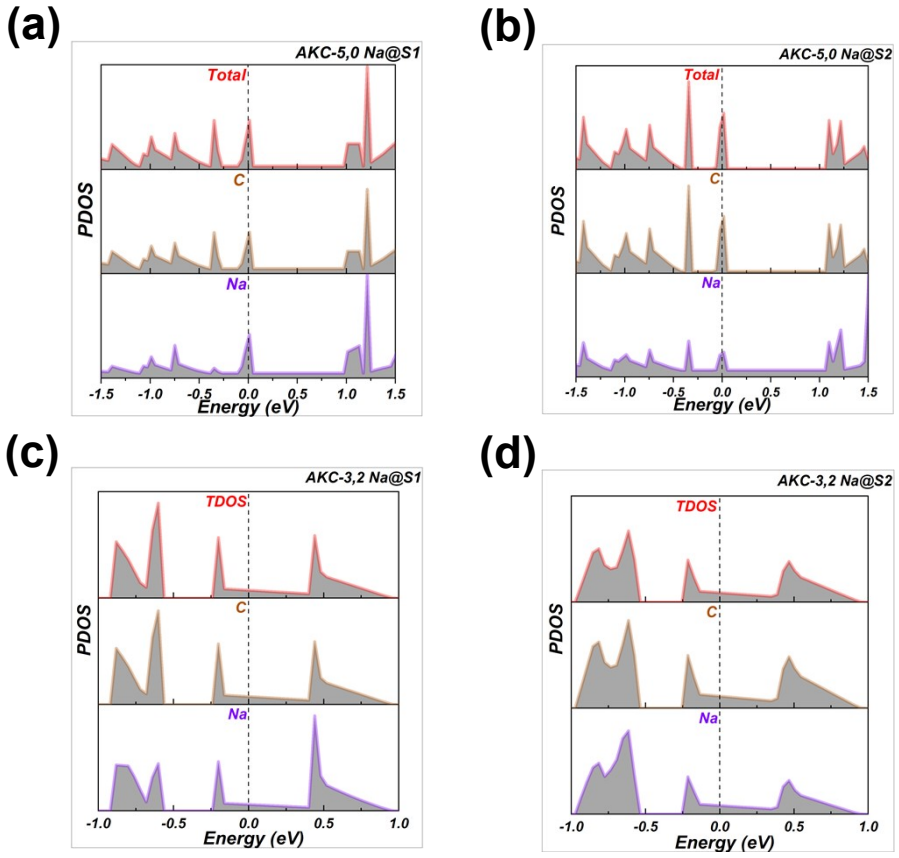

Figure. S3 The partial density of states at the first two adsorption sites for metallic (a-b) AKC-5,0 and (c-d) AKC-3,2 carbon allotropes.

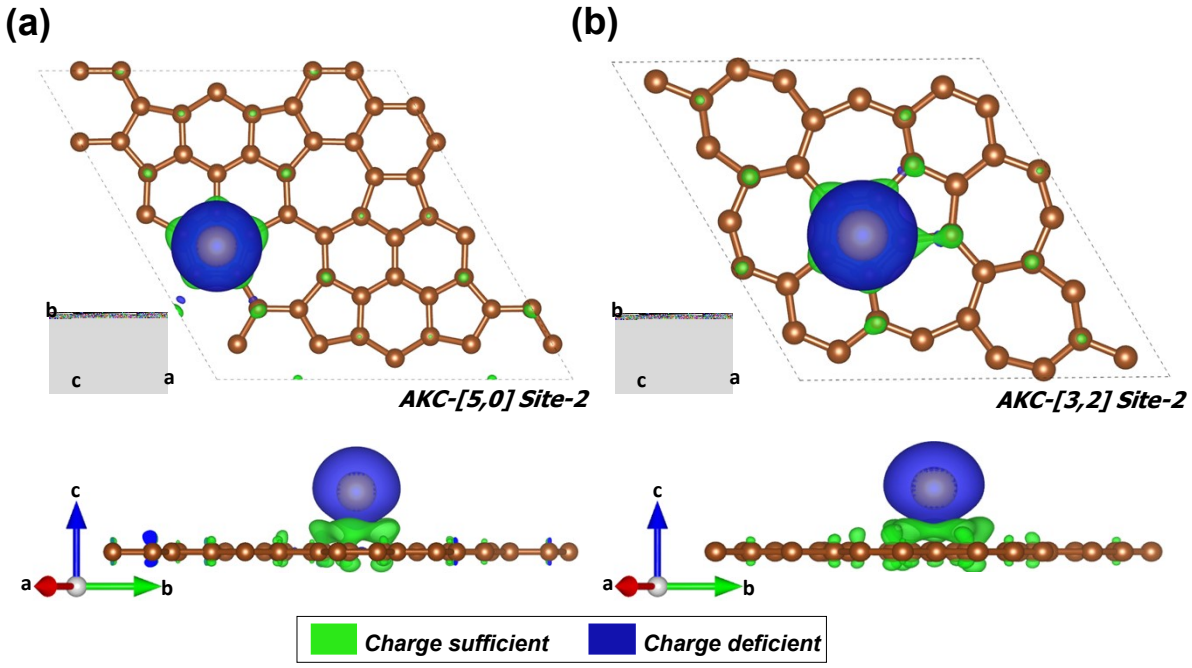

Figure. S4 Results for charge density difference at the second most stable adsorption site of metallic (a) AKC-5,0 and (b) AKC-3,2 allotropes for sodium ion. The green and blue boxes represent the charge sufficient and charge deficient.

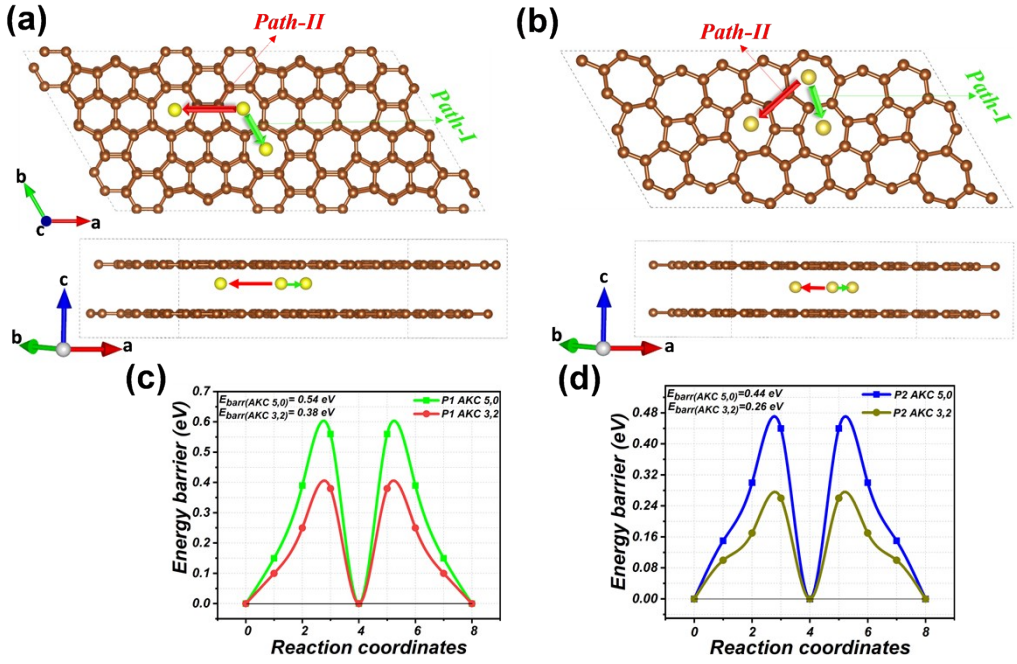

Figure. S5 The two different diffusion pathways for sodium ions over (a-b) bilayer AKC-5,0 and bilayer AKC-3,2 allotropes and (c-d) their respective diffusion profiles.

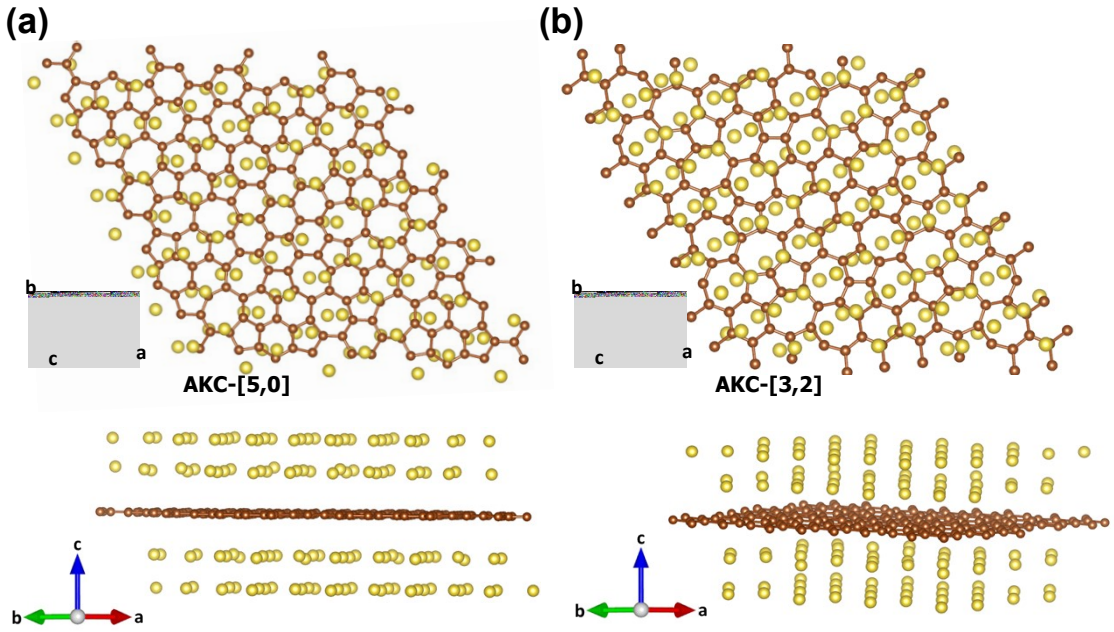

Figure. S6 Top and side view of fully sodiated metallic (a) AKC-5,0 and (b) AKC-3,2 carbon allotropes

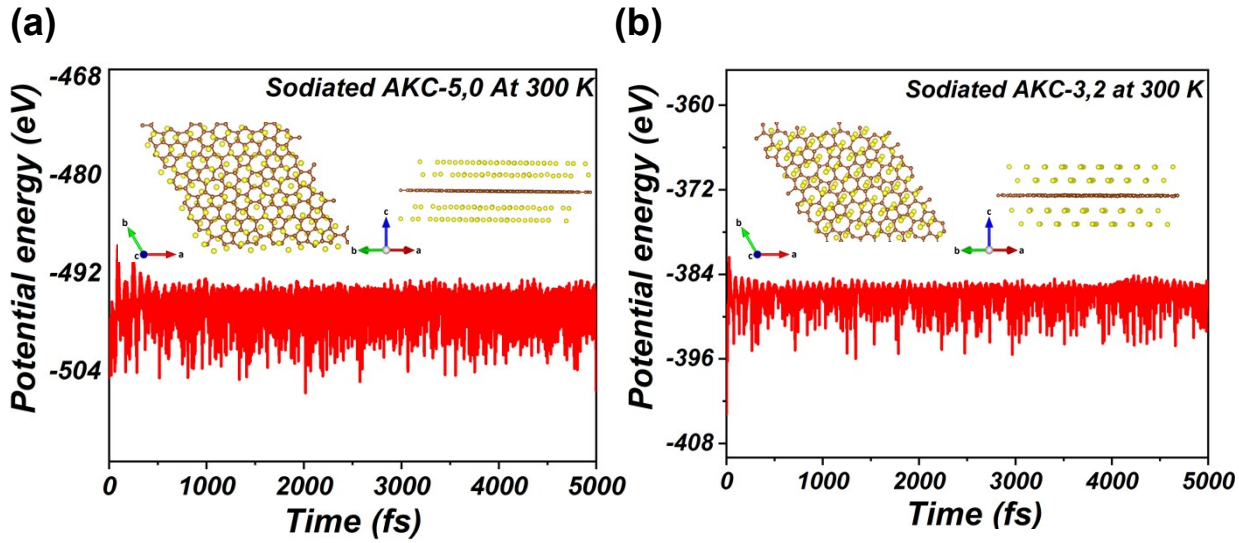

Figure. S7 The fluctuation in potential energy for the fully sodiated metallic (a) AKC-5,0 and (b) AKC-3,2 allotropes with structural distortion calculated at 300 K.

Table. S1 The vibration frequency, zero point energy and energy contribution of Na-ion at T.S for monolayer AKC-5,0 and AKC-3,2 allotropes.

	AKC-3,2		*AKC-5,0*	
	Path-1	*Path-2*	*Path-1*	*Path-2*
Frequency	*117.34 cm-1*	*78.98 cm-1*	*40.86 cm-1*	*53.76 cm-1*
Zero point energy	*0.0186 eV*	*0.0140 eV*	*0.0152 eV*	*0.0161 eV*
Energy contribution at T.S	*0.077 eV*	*0.024 eV*	*0.0896 eV*	*0.0882 eV*