Electronic Supplementary Information (ESI)

Assessing electrochemical properties and diffusion dynamics of metal ions (Na, K, Ca, Mg, Al and Zn) on C_2N monolayer as anode material for non-lithium ion batteries

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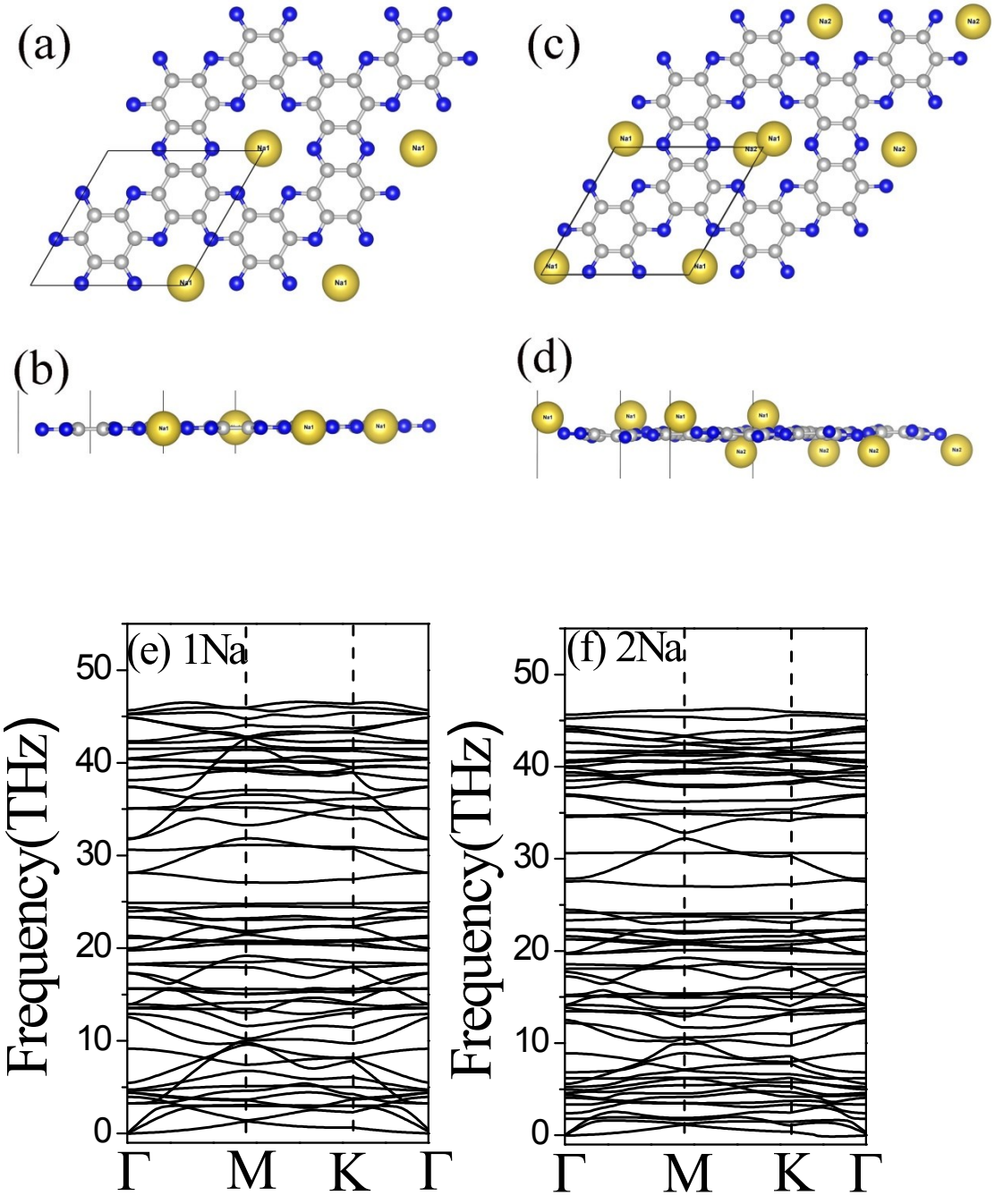

Fig. S1.The first (a and b) and second (c and d) metal atom deposited on C_2N monolayer. The phonon spectra adsorped first (e) and second (f) Na atom of C_2N monolayer along high symmetry directions. First Brillouin zone with the special kpoints: Γ (0.0,0.0,0.0), M (0.5, 0.0, 0.0), K (0.33, 0.33, 0.0), and Γ (0.0, 0.0, 0.0).

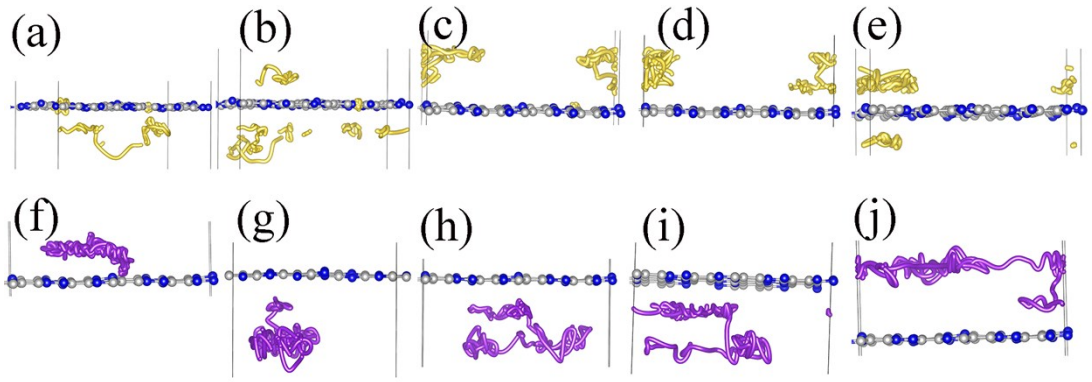

Fig S2 The obtained diffusion pathways of the different Na (a-e) and K(f-j) ion for the C_2N monolayer from the FPMD simulations at 400 K.

Table.S1 The predicted adsorption energies for a single non-lithium atom on C_2N monolayer at stable adsorption sites.

		adsorption energies (No spin calculation)	adsorption energies (Spin calculation)
Na	H_{C-N}	-1.05	-1.09
	H_{C-C}	-0.36	-0.40
	H_1	-3.65	-3.65
K	H_{C-N}	-1.33	-1.38
	H_2	-3.93	-3.93
Mg	H_{C-N}	-0.58	-0.58
	H_1	-5.43	-5.43
Ca	H_2	-4.65	-4.67
Al	H_1	-0.04	0.01
Zn	H_1	-0.07	-0.07