Effect of water molecules on the diffusion of alkali metal ions in CuHCF cathode

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Supporting Information



Figure S1. Simplified schematic diagram of the p-CuHCF structure. Carbon (C) and nitrogen (N) atoms in the structure are omitted. The vertices connected by blue bonds represent the positions of copper (Cu) atoms, while those connected by yellow bonds represent the positions of iron (Fe) atoms.



Figure S2. Schematic diagram of the location of Li^+ , Na^+ , K^+ and H_2O in a unit cell of cubic CuHCF.

Table	S1.	Information	on	the	location	of Li ⁺	, Na+,	K^+	and	H_2O	in	CuHCF	with
[Fe(Cl	N) ₆]	vacancy. W	nere	the p	position o	f O ato	m is re	pres	sents	the po	ositi	ion of H ₂	О.

atom	position	Х	У	Z
Li	32f	0.15	0.15	0.15
Na	32f	0.18	0.18	0.18
K	32f	0.22	0.22	0.22
H ₂ O	24e	0.25	0.5	0.5



Figure S3. From top to bottom, the positional relationships of (a) Li^+ , (b) Na^+ , and (c) K^+ respectively with a water molecule intercalated in p-CuHCF.



Figure S4. Schematic diagram of the location of (a) Li, (b) Na, and (c) K in v-CuHCF.



Figure S5. The diffusion pathway of a single water molecule when there is (a) one, (c) two, and (e) nine water molecules in a vacancy-free supercell. (b), (d) and (f) correspond to the energy barrier diagrams for (a), (b) and (c).



Figure S6. Schematic diagram of two diffusion pathways of (a) single coordination water and (c) single zeolite water in the vacancy-containing supercell. (e) Diffusion of a single zeolite water diffuse from perfect cavities into empty spaces. (b), (d) and (f) are energy barrier diagrams corresponding to the above three migration paths.



Figure S7. (a) Diffusion schematic of a single water molecule (the one with a red oxygen atom, while other non-diffusing water molecules feature pink oxygen atoms) within a supercell containing two to five water molecules. (b) The corresponding diffusion barriers of (a).



Figure S8. In a supercell without vacancy (a) Schematic representation of K^+ diffusion and (b) K^+ diffusion alone when it coexists with water molecules. In a supercell containing vacancy (c) Schematic of K^+ diffusion and (d) K^+ diffusion alone in the presence of water and potassium ions. The direction of diffusion is from left to right in both cases.