

Supporting Information

Achieving robust immobilization of CoP nanoparticles in cellulose nanofiber networks-derived carbon via chemical bonding for stable potassium-ion storage

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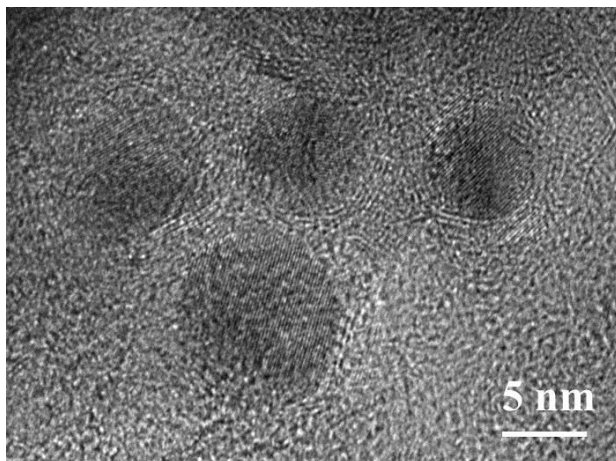


Fig. S1 TEM image of the CoP@CNFC composite.

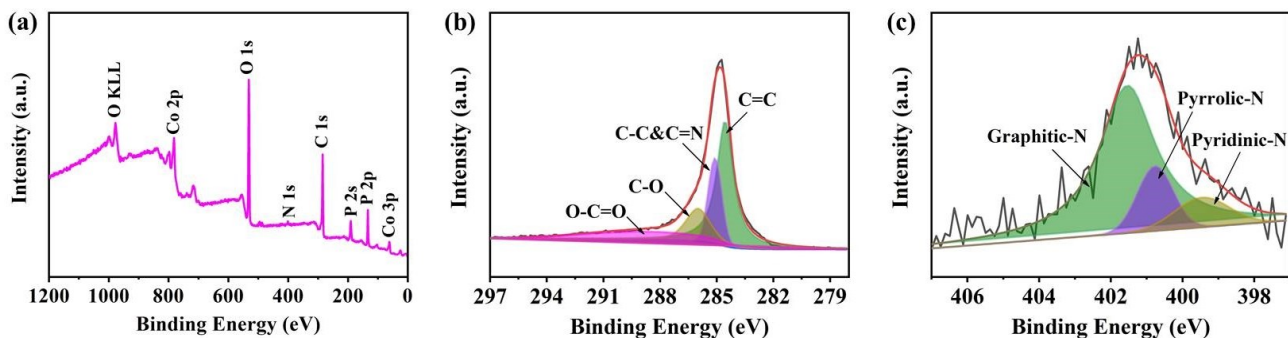


Fig. S2 (a) X-ray photoelectron spectroscopy (XPS) spectra of CoP@CNFC. (b) High-resolution C 1s. (c) High-resolution N 1s.

Table S1 Elemental content analysis result of the CoP@CNFC composite

Elements	Atomic Mass	Atomic Percentage (at%)	Mass content (wt%)
C	12.01	43.14	28.0
N	14.00	1.40	1.10
Co	58.93	6.23	19.8
P	15.98	10.76	18.0
O	16.00	38.46	33.1

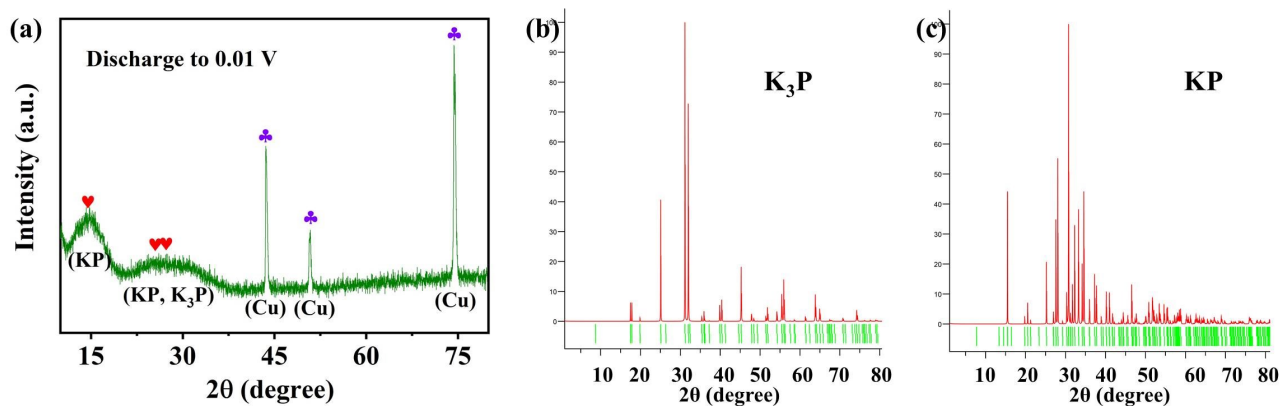


Fig. S3 (a) *Ex-situ* XRD patterns of the electrode discharged to 0.01 V. (b, c) the corresponding XRD patterns of the generated K₃P and KP at the fully discharged stage (0.01V).

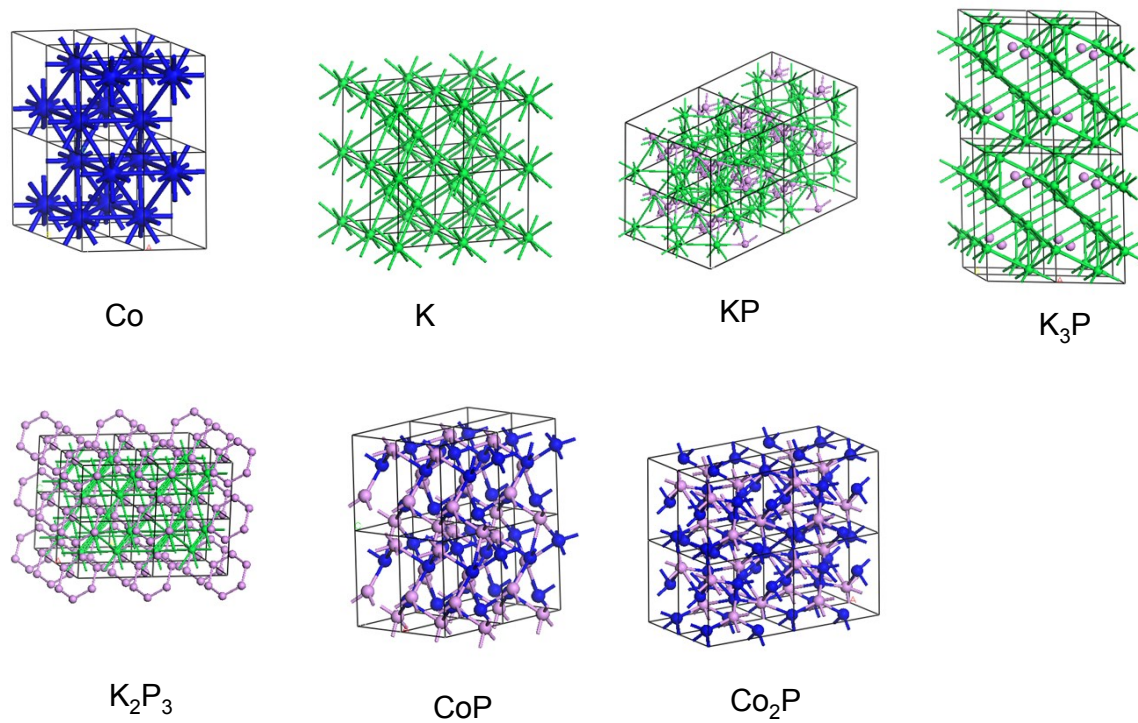


Fig. S4. Optimized bulk species related to the CoP-K-ion battery at the PBE level. Color code: green = K, pink = P, and blue = Co.

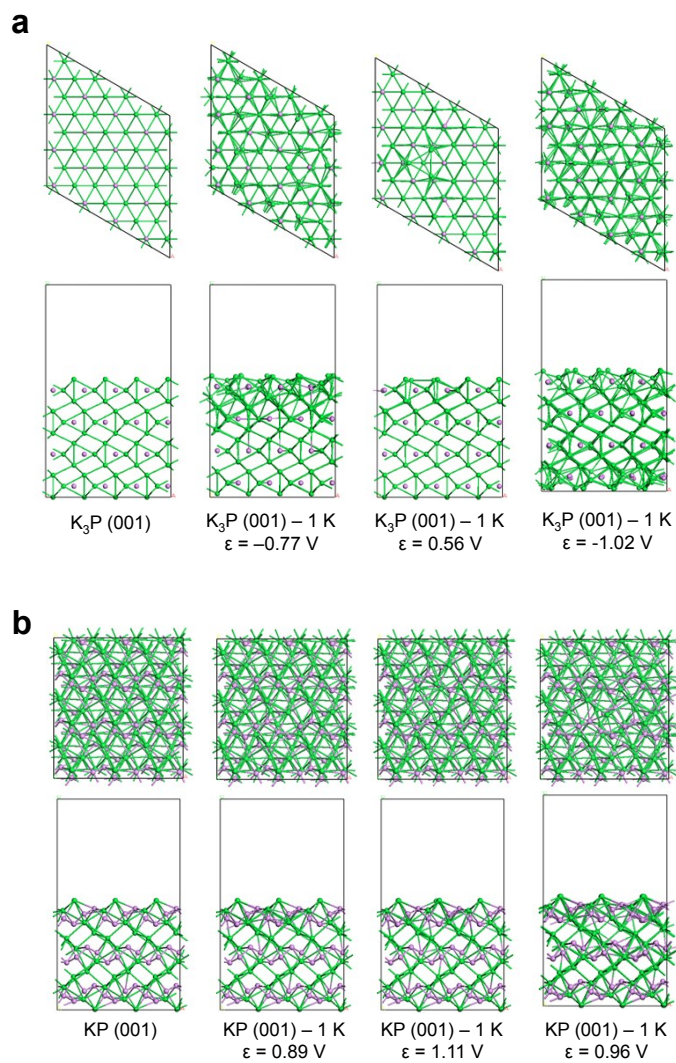
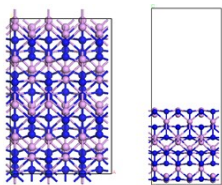
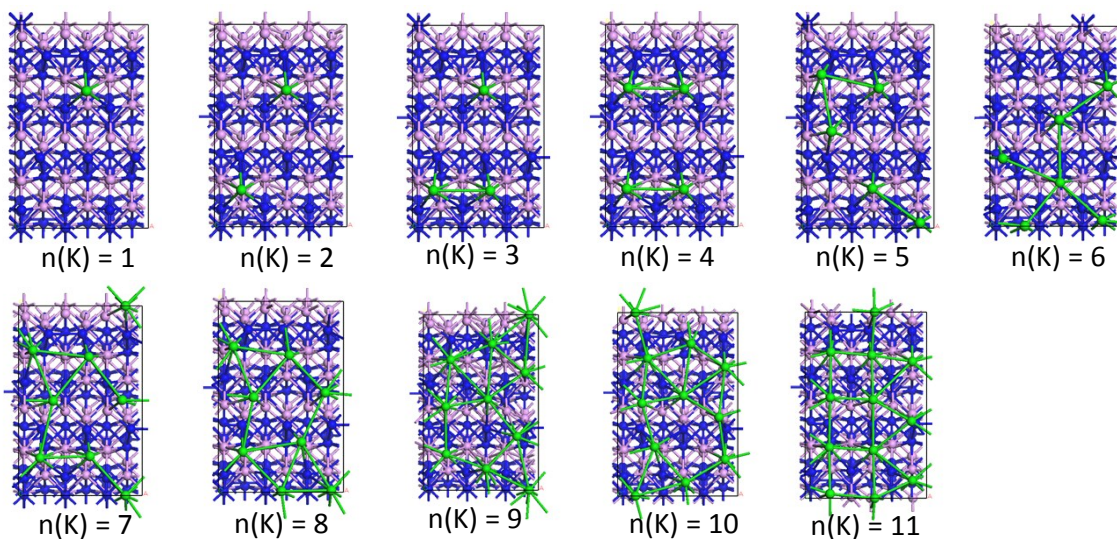


Fig. S5. Optimized geometries and predicted reduction potentials vs. K^+/K for (a) K_3P (001) and (b) KP (001) surfaces at the PBE level. Color code: green = K, and pink = P.

CoP (011):



K-coverage \leq monolayer:



K-coverage $>$ monolayer:

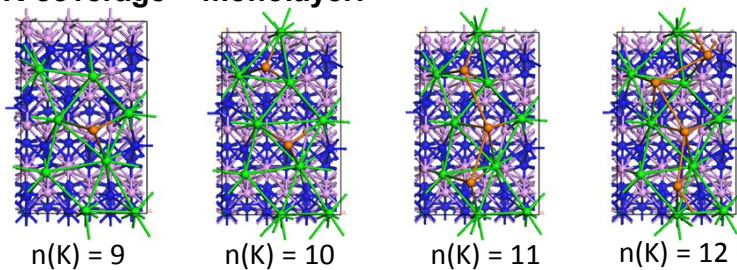


Fig. S6. Optimized geometries for potassiation of the CoP(011) slab. The surface area of the slab is 147.0 \AA^2 . Color code: green = K (first layer), orange = K (second layer), pink = P, and blue = Co.

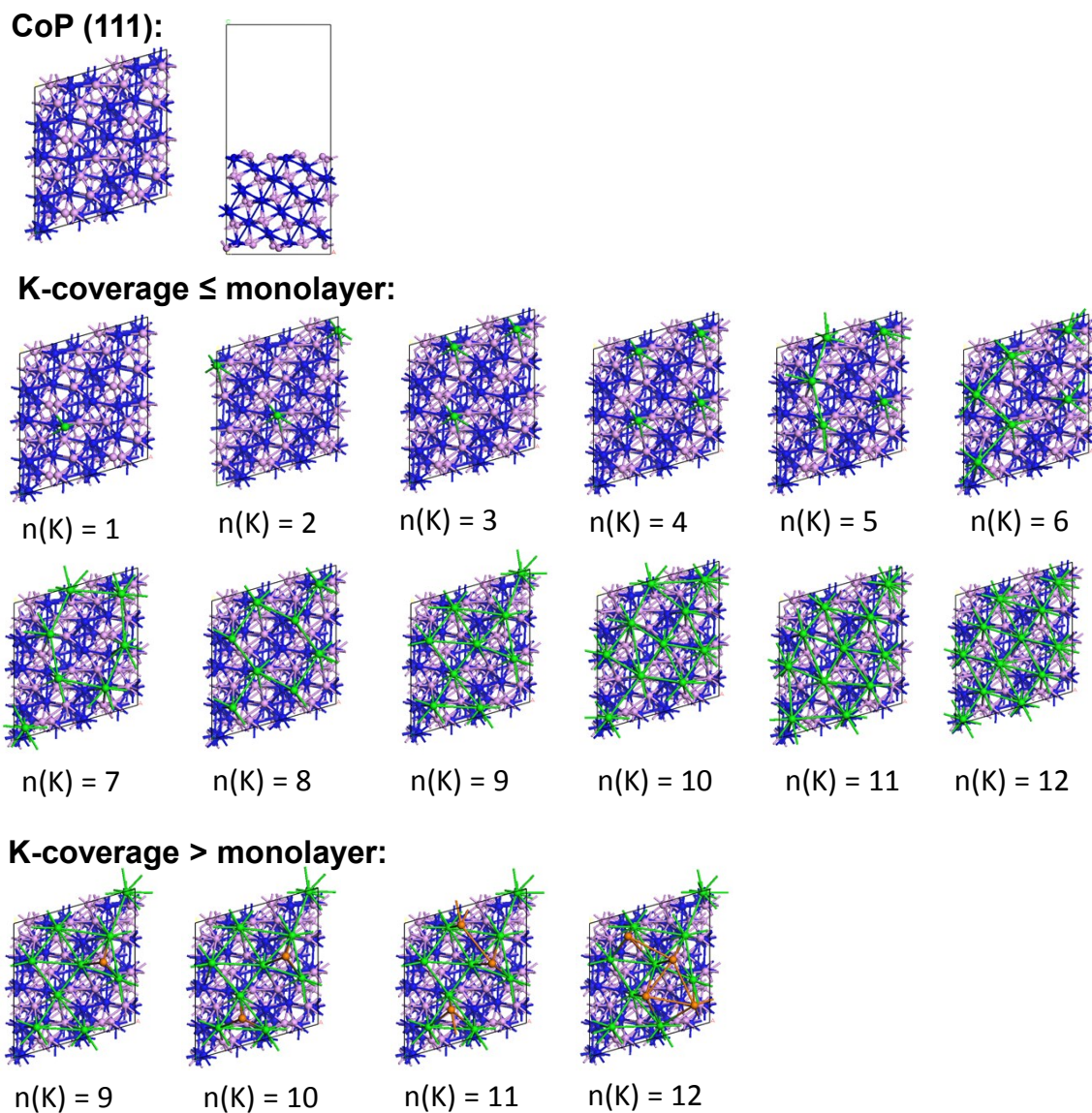


Fig. S7. Optimized geometries for potassiation of the CoP(111) slab. The surface area of the slab is 148.9 \AA^2 . Color code: green = K (first layer), orange = K (second layer), pink = P, and blue = Co.

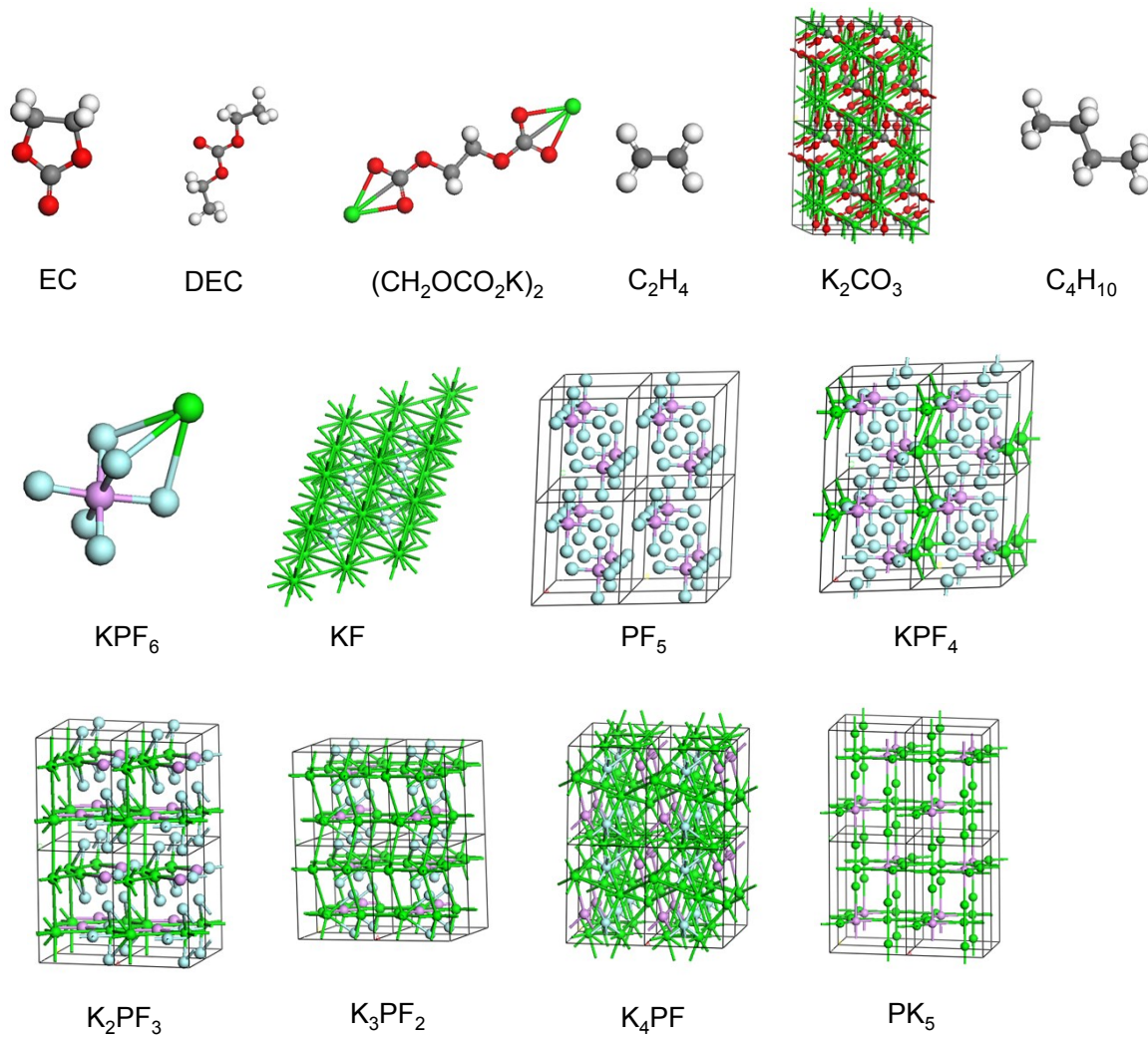


Fig. S8. SEI-related Species for K-ion battery with EC, DEC, and KPF_6 electrolytes.