

Supporting Information

Copper Phosphide: A high volumetric capacity anode material for Potassium-ion batteries

Qiuran Yang^a, Zhixin Tai^a, Qingbing Xia^a, Weihong Lai^a, Wanlin Wang^a, Binwei Zhang^a, Zichao Yan^a, Jian Peng^a, Huiling Yang^a, Hanwen Liu^a, Qinfen Gu^b, Shulei Chou^{*a}, Huakun Liu^a

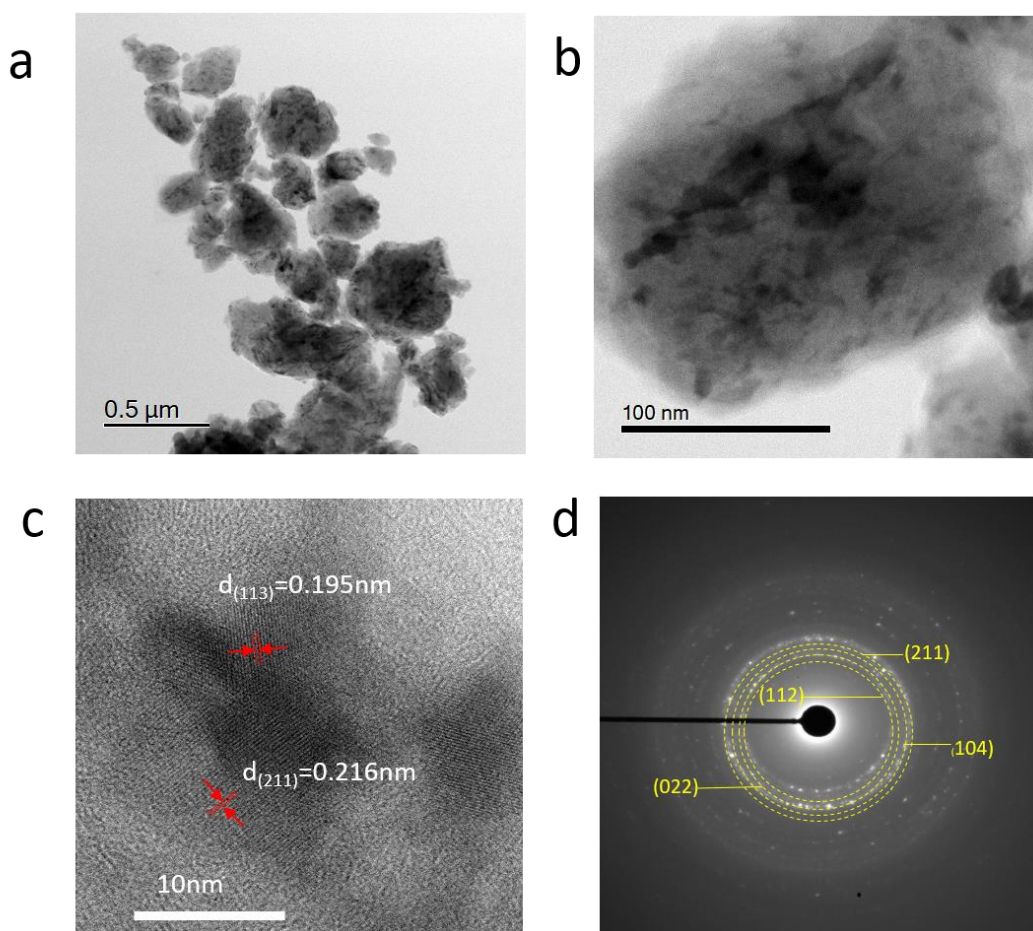


Figure S1. Transmission electron microscope (TEM) analysis of CPS. (a-c) HRTEM images and (d) SAED pattern.

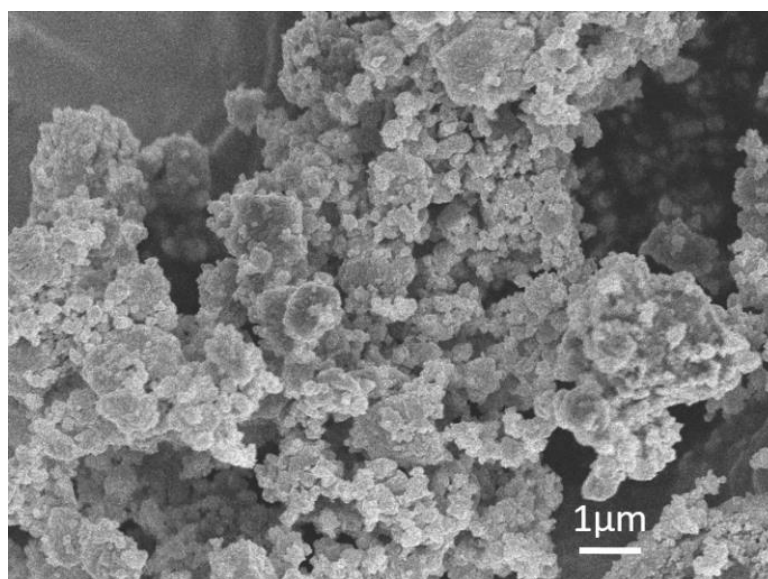


Figure S2. SEM image of CPS.

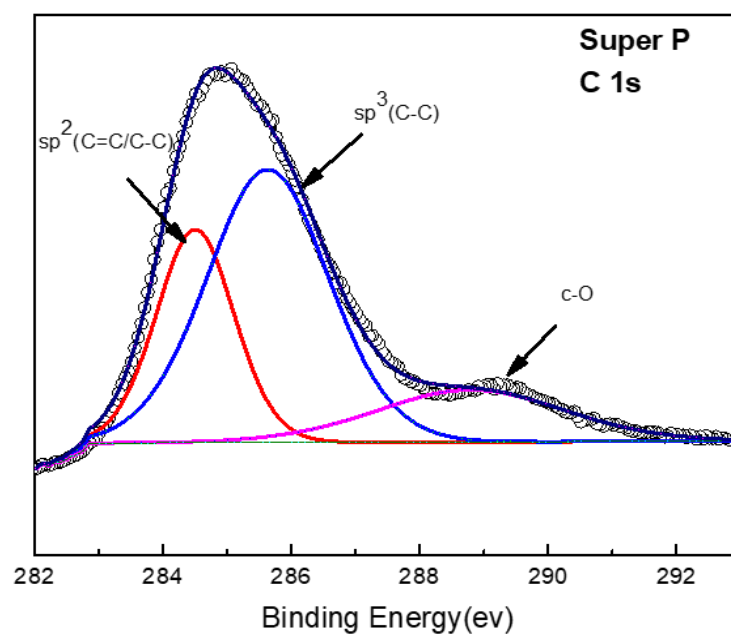


Figure S3. XPS survey spectra of the carbon black.

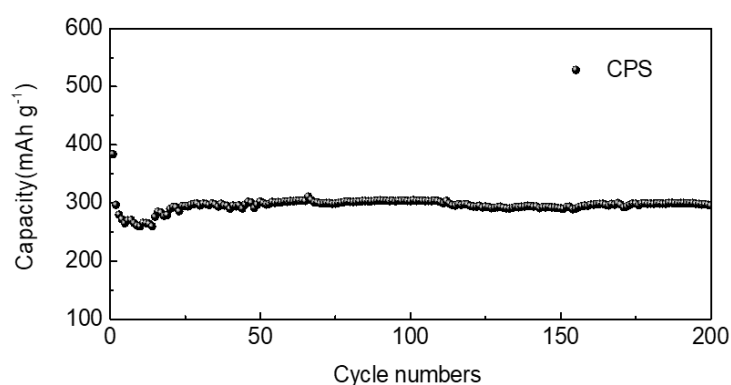


Figure S4. cycling performance of CPS at current density of 100 mA g⁻¹.

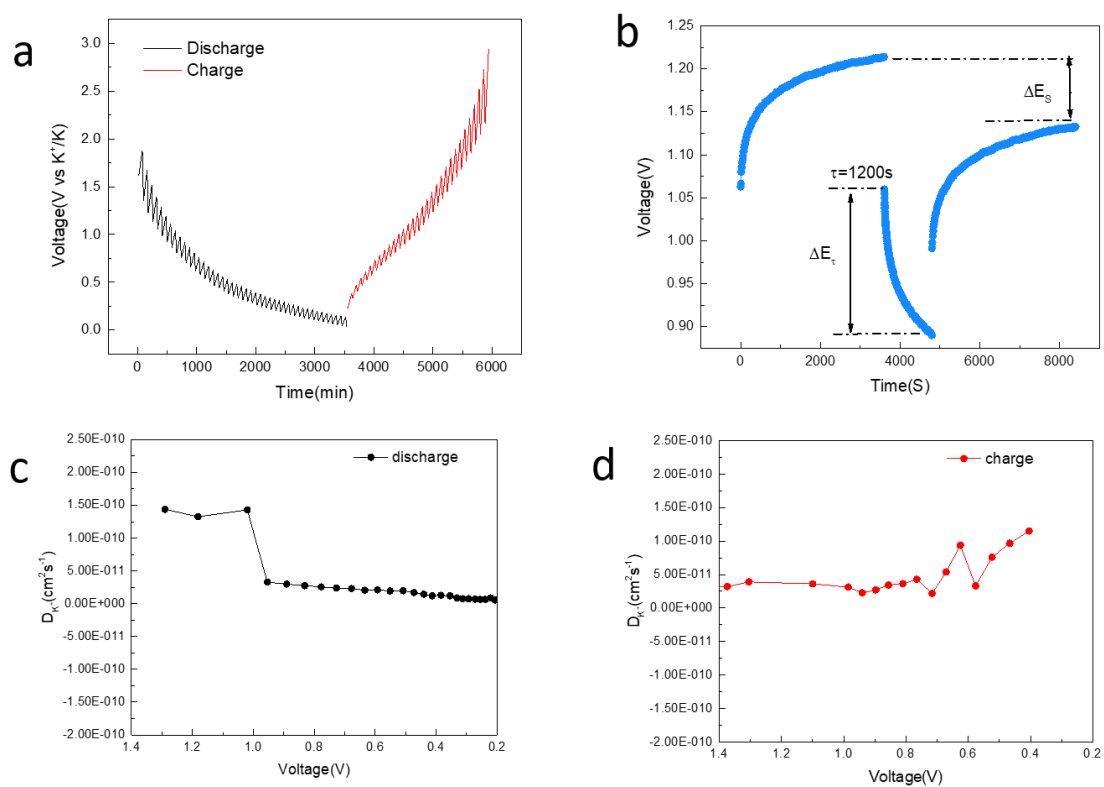


Figure S5. (a) GITT profiles during charge for the CPS electrode in the voltage window of 0-3 V. (b) Voltage vs. time for a single titration step in GITT. Calculated K⁺ ion diffusion coefficient of CPS during (c) discharge and (d) charge processes.

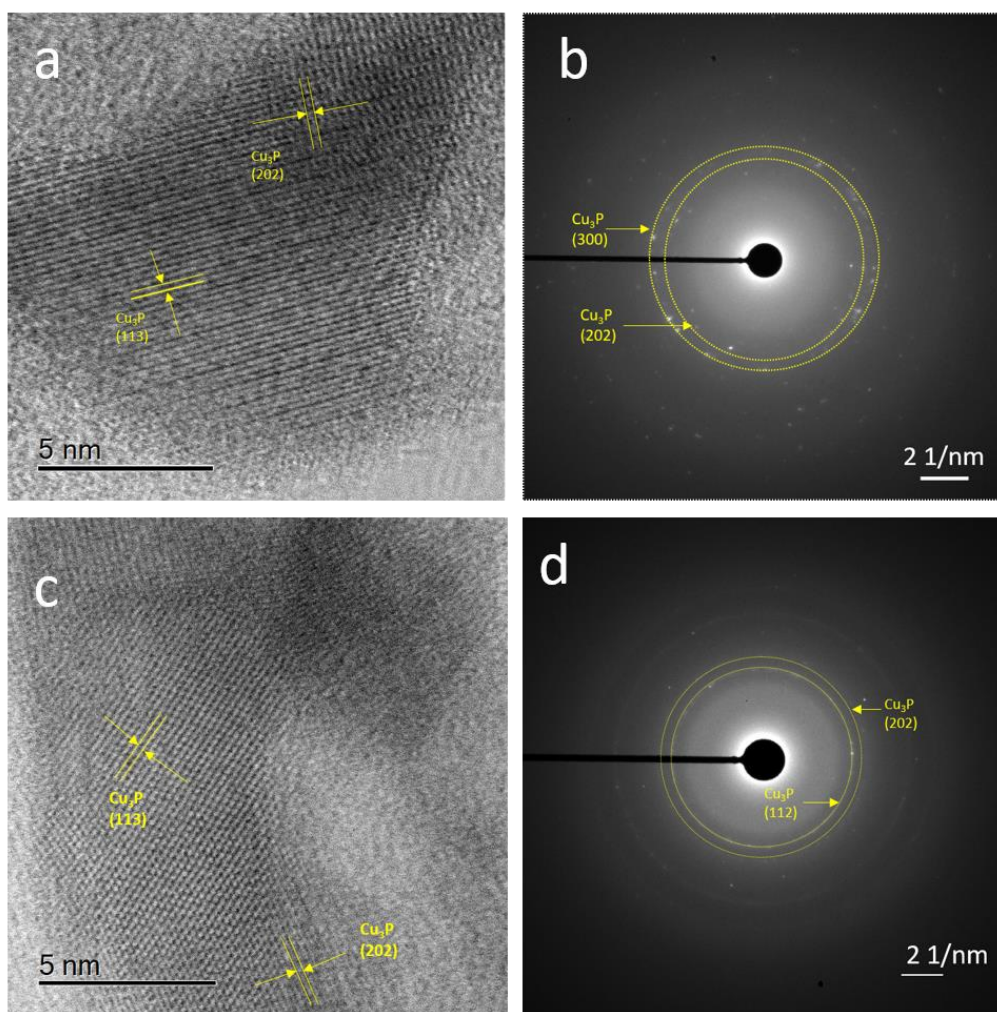


Figure S6. (a) HRTEM image and corresponding SAED diffraction pattern of the electrode discharged to ①. (c) HRTEM image and corresponding (d) SAED diffraction pattern of the electrode charged to ④. The numbers refer to points on the charge-discharge curve in Fig. 5a.

Table S1 Detailed structural information on the CPS sample after Rietveld refinement.

CPS(Cu ₃ P). Hexagonal, space group P6 ₃ cm, $a = b = 6.952306 \text{ \AA}$, $c = 7.137323 \text{ \AA}$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$ $V = 298.761 \text{ \AA}^3$, $R_{wp} = 3.309\%$					
Atom	x	y	z	Site	Occupation
Cu1	0.28476	0.00000	0.07466	6c	1
Cu2	0.37076	0	0.42533	6c	1
Cu3	0.33330	0.66670	0.20257	4b	1
Cu4	0.00000	0.00000	0.31559	2a	1
P	0.33501	0.00000	0.75495	6c	1