Supporting Information

Microstructure and Charge–Discharge Mechanism of a Li_3CuS_2 Positive Electrode Material for All-Solid-State Lithium-Ion Batteries

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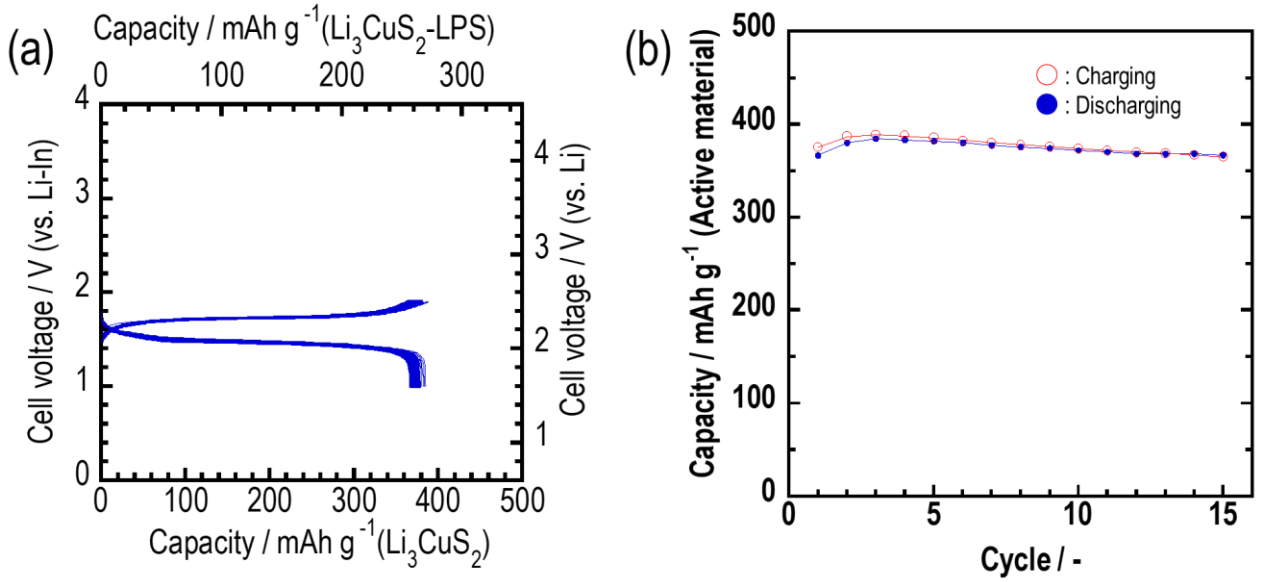

Fig. S1 Charge−discharge properties of Li−In/LPS/Li_3CuS_2−LPS cells fabricated in the present study. (a) Charge−discharge curves of the cell. (b) Cycling stability of the cell.

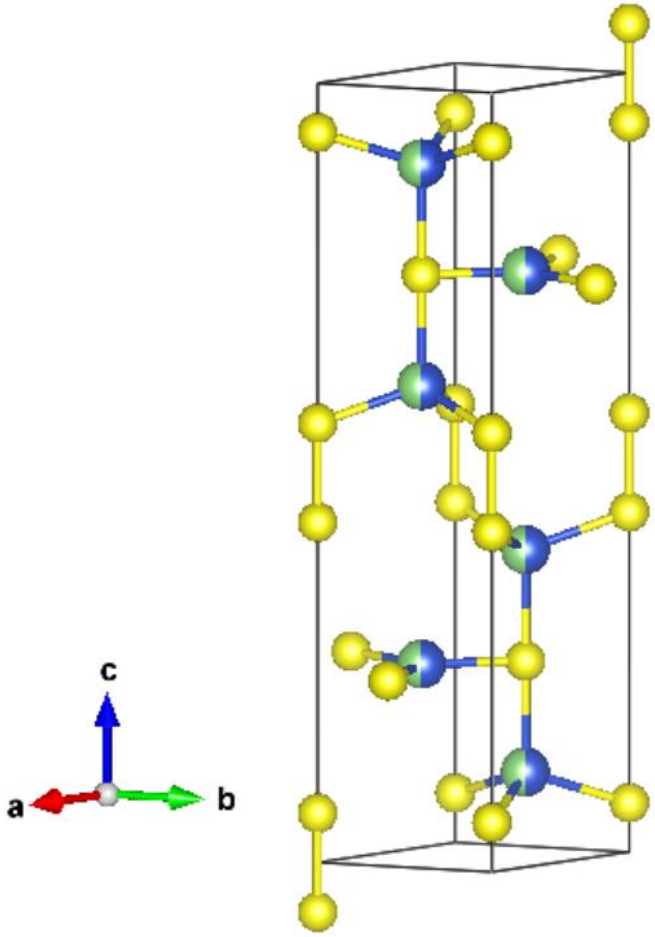

Fig. S2 Crystal structure of cation-disordered $P6_3/mmc$ $LiCuS_2$ (CuS-type structure).

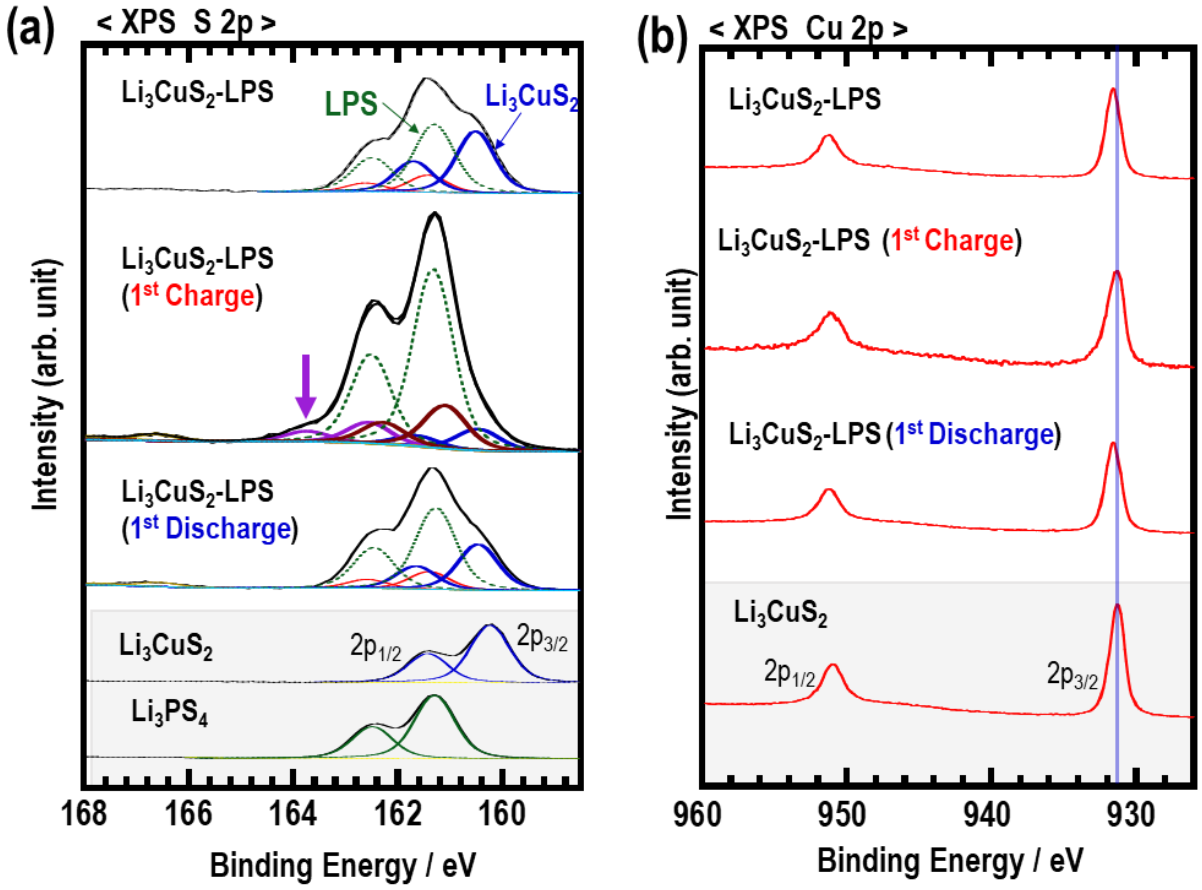

Fig. S3 (a) S 2p XPS spectra of Li_3CuS_2–LPS composites before and after charge–discharge cycles. The green dotted lines are the peaks attributed to LPS in the composites. The half widths of the LPS S 2p peaks in the composites are the same as that of a single-phase LPS S 2p peak. The S 2p peak areas of LPS in the composites are defined from the peak area ratio (S 2p/P 2p) of the single-phase LPS and the P 2p peak areas of the composites (Fig. S4). The S 2p peaks, shown in red, are probably due to the sulfur states near the Li_3CuS_2/LPS interface. (b) Cu 2p XPS spectra of the composites.

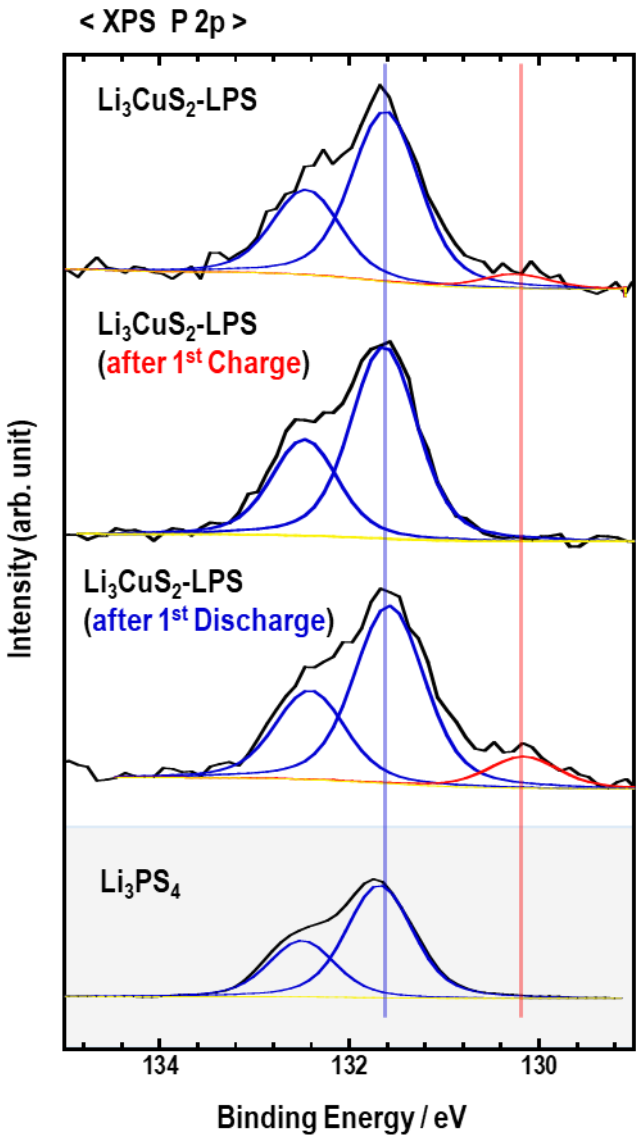

Fig. S4 P 2p XPS spectra of Li_3CuS_2–LPS composites before and after the initial charge–discharge cycles. For the main blue peaks, peak shift is not observed before and after charging and discharging. Thus, most of the LPS is not involved in redox reaction. The red P 2p peaks are attributed to the phosphorus states near the Li_3CuS_2/LPS interfaces. The red P 2p peak disappeared after the initial charge and reappeared after the discharge. This implies that LPS is partially involved in redox reaction.