Electronic Supplementary Information

Crystal structure and electrical/thermal transport properties of $Li_{1-x}Sn_{2+x}P_2$ and its performance as a Li-ion battery anode material

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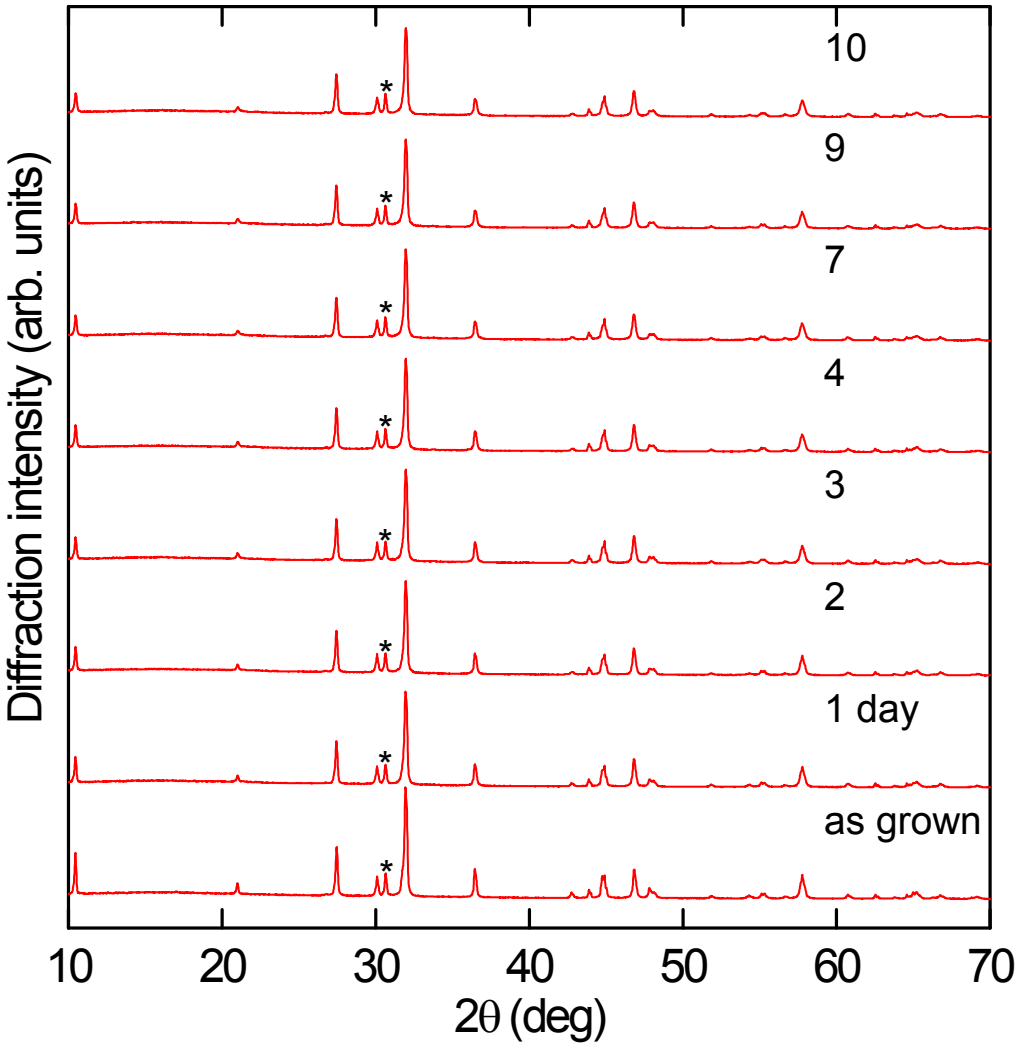

Figure S1

XRD patterns of $Li_{1-x}Sn_{2+x}P_2$ exposed to air for 10 days without any visible signs of oxidation/hydrolysis. Asterisk denote the diffraction peak due to Sn_4P_3.

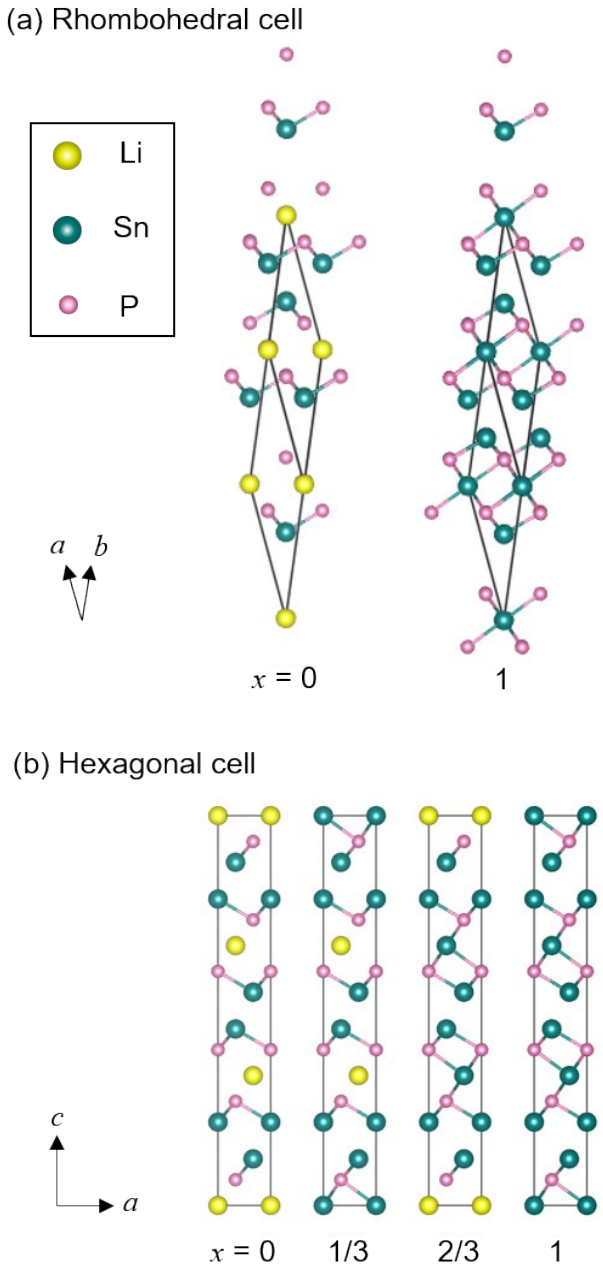

Figure S2

Crystal structures of $Li_{1-x}Sn_{2+x}P_2$ used for first-principles calculations with (a) rhombohedral and (b) hexagonal cells.

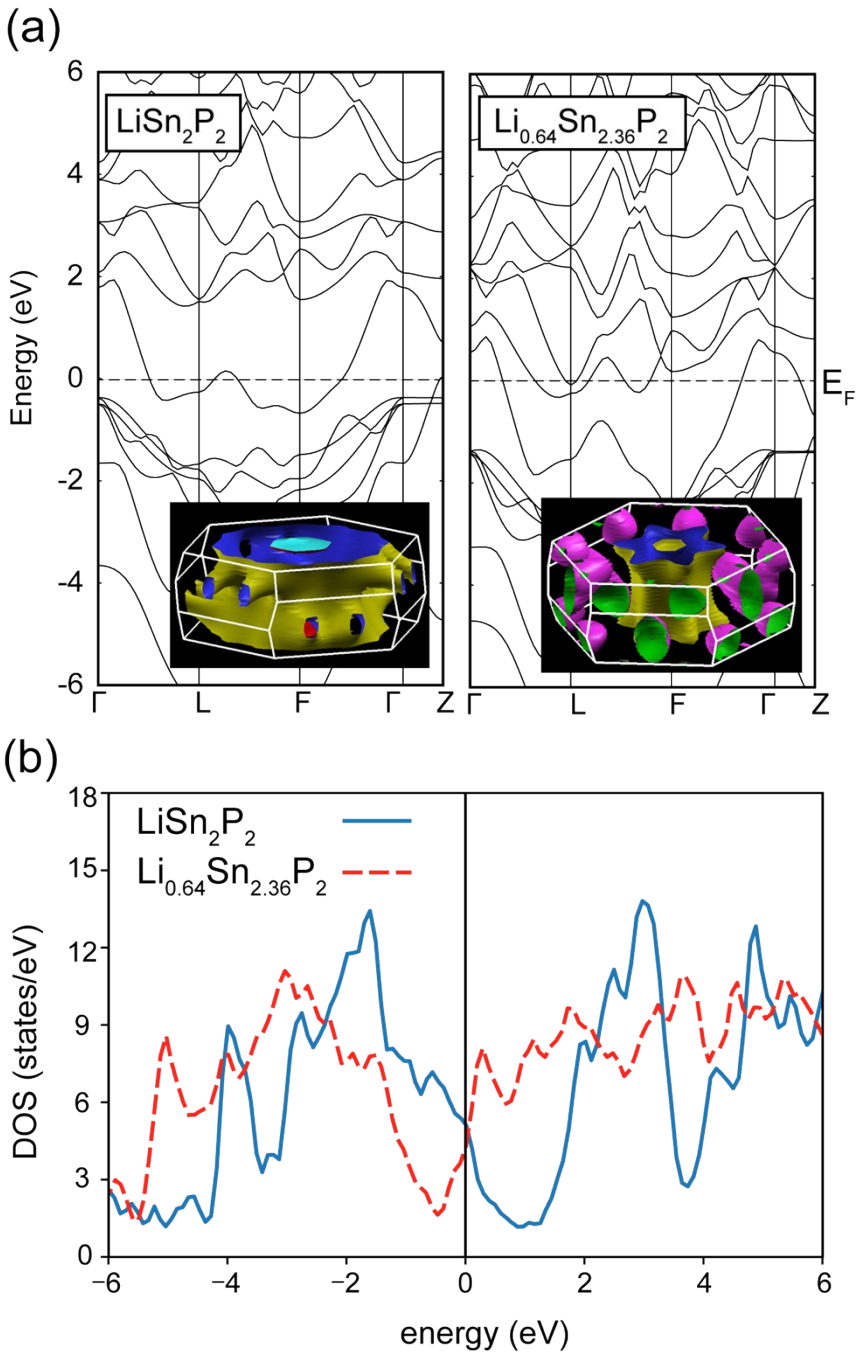

Figure S3

(a) The electronic band structure and the Fermi surface (inset), and (b) the density of states of $Li_{1-x}Sn_{2+x}P_2$ calculated within the virtual crystal approximation.