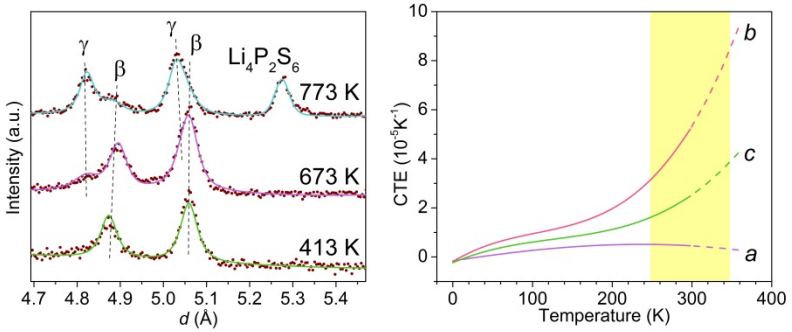
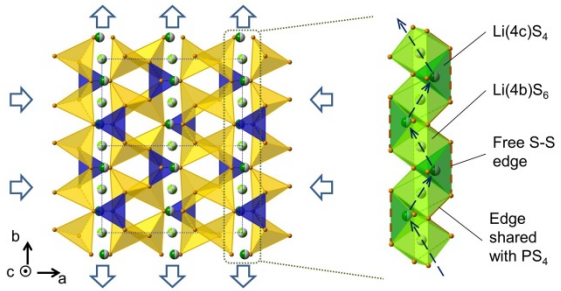
Correlation of anisotropy and directional conduction in β-Li_3PS_4 fast Li^+ conductor





Neutron and X-ray diffractions determine the stability of β-Li_3PS_4 and the anisotropic thermal expansion with its structural origin from Li^+ channels.

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Scientific Achievement

The β-Li_3PS_4 is found to have strong anisotropy of thermal-strain response, structurally correlated with the directional ionic transporting channels.

Significance and Impact

This work provides important considerations of thermal stability, physical compatibility and optimization of ionic transport in the solid electrolyte, for next-generation all-solid-state batteries that adapt to a wider temperature range of operation to deliver larger power.

Research Details

- Neutron and X-ray powder diffraction determine the crystal structure and thermal stability.
- In-situ diffraction reveals a fast expansion direction along the crystallographic *b*-axis while a negligible expansion along the *a*-axis in response to heating.
- The anisotropic behavior has its structural origin from the Li^+ conduction channels with incomplete Li occupancy and a flexible connection of LiS_4 and PS_4 tetrahedra in the framework.

Y. Chen, L. Cai, Z. Liu, C. R. dela Cruz, C. Liang, and K. An, Applied Physics Letters **2015**, 107, 013904.