

MS43-04 | USING NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY, NEUTRON AND X-RAY PAIR

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To develop all-solid-state batteries it is crucial to understand the structure property relationship in solid-state electrolytes (SE). However, freely after the quote of Wolfgang Pauli: *“The best that most of us can hope to achieve in physics is simply to misunderstand at a deeper level”*, our knowledge of the real structure of SEs remains oversimplified. Nonetheless, it is crucial to understand the role of defects and distortions in these materials in detail, since such structural peculiarities highly correlate with ion migration. Like many promising SE candidates, the argyrodites $\text{Li}_6\text{PS}_5\text{X}$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) are built up by isolated polyhedral species, in this case $[\text{PS}_4]^{3-}$ tetrahedra. A review of the effect of lattice distortions and ion migration barriers revealed a discrepancy between proposed mechanisms for argyrodites and other solid state electrolytes, indicating that the defect structure is not well understood yet. Our Neutron and X-Ray PDF study of $\text{Li}_6\text{PS}_5\text{Cl}$, revealed that the low r region ($< 5 \text{ \AA}$) of the PDF could not be satisfactorily fitted using a cubic model, mainly due to the strongly increased peak corresponding to S – S distances within $[\text{PS}_4]^{3-}$ tetrahedra and a missing peak corresponding to inter-tetrahedra $\text{S}_{\text{tet}} - \text{S}_{\text{tet}}$ distances. Although it is possible to use models with reduced symmetry to fit the low r region better, we have strong indications that this is still an oversimplified model to the real structure.