Characterizing diffusion channels in lithium thiophosphate glassy electrolytes

Christensen, Rasmus; Biscio, Christophe; Fajstrup, Lisbeth; Smedskjær, Morten Mattrup

Publication date:
2022

Document Version
Other version

Characterizing diffusion channels in glassy electrolytes using topological data analysis

R. Christensen[1*], C. Biscio[2], L. Fajstrup[2], M. M. Smedskjaer[1]

[1] Department of Chemistry and Bioscience, Aalborg University, DK-9220 Aalborg, Denmark.,
[2] Department of Mathematical Sciences, Aalborg University, DK-9220 Aalborg, Denmark.
*rasmusc@bio.aau.dk

Identifying solid electrolytes with high ionic conductivity at room temperature is critical for designing solid state batteries with high safety and energy density relative to conventional liquid-based batteries. Lithium thiophosphate glasses are considered to be potential electrolyte materials due to their high Li^+ ion conductivity. However, understanding of the Li^+ ion conduction mechanism in these materials is limited due to the complex nature of their disordered structures. To investigate the Li^+ ion conduction mechanism, we here evaluate a series of lithium thiophosphates [x Li_2S – (100 - x) P_2S_5] based on ab initio molecular dynamics simulations. We then employ persistent homology, an emergent type of topological data analysis, to analyse the generated structures. This method is used to characterize the geometry and composition of the lithium diffusion channels, both in static structures and in structures that develop over time. To this end, we investigate how the structural units present in the glasses can be coupled to their ionic conductivity and whether these structures can be tuned to enhance the ionic conductivity.