# Analyzing lithium ion conductivity in thiophosphate glassy electrolytes via machine learning

Chen, Zhimin; Du, Tao; Christensen, Rasmus; Bauchy, Mathieu; Smedskjær, Morten Mattrup

*Publication date:*
2023

# Analyzing lithium ion conductivity in thiophosphate glassy electrolytes via machine learning

**Zhimin CHEN[1], Tao DU[1], Rasmus CHRISTENSEN[1], Mathieu BAUCHY[2], and Morten M. SMEDSKJAER[1,*]**

*[1] Department of Chemistry and Bioscience, Aalborg University, Aalborg East 9220, Denmark, mos@bio.aau.dk*

*[2] Department of Civil and Environmental Engineering, University of California, Los Angeles, CA, 90095, USA*

Glasses such as lithium thiophosphates ($Li_2S$-$P_2S_5$) show promise as solid electrolytes in lithium-ion batteries, but a poor understanding of the mechanism by which the disordered structure affects lithium transport properties limits the development of glassy electrolytes. To address this, we here simulate glassy $Li_2S$-$P_2S_5$ electrolytes with varying fractions of polyatomic anion clusters using classical molecular dynamics. Based on the determined variation in ionic conductivity, we use a classification-based machine learning metric termed “softness” – a structural fingerprint that is correlated to the atomic rearrangement probability – to unveil the structural origin of lithium-ion mobility. To derive a real-space origin of the machine-learned softness metric, we analyze the energy barrier of softness-coded lithium ions migrating between two sites, showing that soft lithium-ion migration requires a smaller energy barrier to be overcome relative to that observed for hard lithium-ion migration.