Contribution ID: **30** Type: **Oral**

Ion dynamics in solid electrolytes for batteries

Wednesday, 14 September 2022 09:00 (45 minutes)

Fast ion-conductors, especially those conductive for lithium and sodium cations, have been the subject of intense (re)investigation lately in the context of electrochemical applications, most notably as solid electrolytes in all-solid-state-batteries. In that context, ions need to travel macroscopically (i.e. in the μm-mm scale) between electrodes to charge and discharge the cell. As such, the main functional property of interest in solid electrolyte materials is macroscopic ionic diffusivity/conductivity, but application to next-generation batteries also imposes a host of other requirements, namely, processability, (electro)chemical- and mechanical stability during operation etc.

In this talk, recent advancements in the fundamental understanding of ion-conduction in solid electrolytes will be elaborated, using topical example materials such as the thiophosphates Na₃PS₄ and Li₃PS₄. The use of multiple complementary spectroscopic probes (neutron-, NMR-, Raman-, impedance- spectroscopies) along with atomistic simulation techniques (molecular dynamics, nudged elastic band) is paramount to obtaining a complete multiscale picture of solid-state ionics, and thus allow for further advancements.

Key outstanding questions will be posed for discussion such as a) the role of harmonic vs. unharmonic dynamics in predicting, understanding and tuning ionic conductivity in solids and b) the interplay between host anion (lattice) dynamics and mobile cation mobility/diffusivity.

Primary author: FAMPRIKIS, Theodosios

Presenter: FAMPRIKIS, Theodosios

Session Classification: Session 4 : Batteries & ionic conductors