Ionic conduction pathways in chalcogenide glasses: experimental evidence and modelling

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Extended R&D in the field of alternative energy sources stimulates studies of all-solid-state lithium and sodium batteries for portable electronics, transport and stationary applications. Chalcogenide vitreous electrolytes and glass/ceramic composites belong to promising functional materials offering record-high ionic conductivity and advanced charge/discharge cycling. The origin of the superionic mobility in a chalcogenide glass remains an open question often related to preferential conduction pathways formed in the disordered network. Using pulsed neutron and high-energy X-ray diffraction combined with RMC/DFT modeling, we will unveil the nature of ionic conduction pathways in glassy chalcogenides. The tracer diffusion experiments and Raman spectroscopy measurements yield an independent verification of the proposed scenario providing a deeper insight into the interesting and practically important phenomenon.

Keywords: ion, conducting chalcogenide glasses, neutron diffraction, high, energy x, ray diffraction, RMC/DFT modelling, tracer diffusion

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