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Structural Drivers of Na diffusion in oxy-thiophosphate amorphous electrolytes. A Machine Learning Molecular dynamics study in the framework of the EcosistER project.

The global growing demand for energy storage is pushing the research for new battery materials with improved performance, safeness, and environmentally friendly synthesis, usage, and disposal. All-Solid-State Sodium Batteries (ASSSB) are attracting increasing attention from both academia and industry as strong candidates for grid-scale energy storage. However, their development requires highly conductive and electrochemically stable Solid-State Electrolytes (SSEs). Among the possible candidates, Glassy Solid Electrolytes (GSEs) are particularly promising as they can potentially meet all the requirements for a good SSE. They can achieve ionic conductivities comparable to those of liquid electrolytes while preventing dendrite growth and fire hazard[1]. Using sodium as a charge carrier allows avoiding the ethical concerns associated with lithium mining and mitigates possible supply chain issues, thanks to the higher Na abundance. The development of ASSSBs needs a huge effort in the study of a suitable SSE. Most of the GSE studied so far are based on sulfide glasses which offer high conductivity but suffer from high reactivity with atmospheric compounds. Recently, mixed oxy-sulfide (MOS) glasses have been explored as a way to combine the chemical stability of oxide glasses with the conductivity of sulfide ones. From a computational perspective, the lack of classical interatomic potentials for these systems limits their structural investigations, as ab-initio methods are constrained by their computational cost. In this work, we developed a Machine Learning Interatomic Potential (MLIP) to study the structure of MOS glasses and correlated it with the Na diffusion[2]. The accuracy and computational efficiency of the MLIP allow us to perform simulations beyond the capabilities of ab-initio methods, identifying structural units that promote or hinder Na diffusion and relating them to the glass composition, thus paving the way for the design of new GSE with tailored properties. This project is funded under the PNRR Miss. 4, Comp. 2, Inv. 1.5, NextGenerationEU-Avviso 3277/2021 – ECS_00000033-ECOSISTER-spk06.

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[2] M. Bertani and A. Pedone, J. Phys. Chem. C, under revision.

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