Contribution ID : **76** Type : **Poster Presentation**

Machine Learning potentials for Amorphous Solid Electrolytes in Sodium All-Solid-State Batteries: investigating the Mixed Glass Former Effect

The topic of solid electrolytes for energy storage systems is both fascinating and crucial from an environmental and sustainability perspective. Liquid electrolytes, commonly made from lithium compounds, face low stability and high cost. Furthermore, lithium extraction is not sustainable for the environment or local communities. Thus, researchers are eager to develop safer and more ecological alternatives. All-solid-state sodium batteries (ASSSBs) are promising candidates for grid- scale energy storage, but there is still much to understand about the electrochemical stability of solid electrolytes with sodium. Amorphous sodium phosphorus sulfides (NPS) show a high critical current density, but they suffer electrochemical instability with electrode materials. To overcome this limitation, while maintaining the conduction properties, the mixed glass former (MGF) effect can be used partially substituting phosphorous with silicon (NPSiS). Previous experimental studies on these compositions, such as those by Shastri et al. [1], have shown that modifying the ratio of these network formers can significantly influence conductivity, but the relationship between their composition, structure, and properties at the atomic level remains unclear. Molecular Dynamics is the most effective computational method to investigate the properties of NPS and NPSiS solid electrolytes: however, studies on these systems are hindered by the lack of classical interatomic potentials, while the high computational cost of ab initio methods limits their feasibility for extensive structural analysis. Machine Learning techniques, instead, offer a promising solution to develop new reliable potentials for various materials. In this work, we developed Machine Learning interatomic potentials (MLIPs) trained on NPSiS compositions. The developed MLIP was used to study how the composition of sodium-based amorphous electrolytes affects their atomic structure and ionic conductivity focusing on the mixed glass former effect given by silicon. The studied compositions are y Na_2S + (1−y) [x SiS_2 + (1−x) PS] with x = 0.5 or 0.67 and y varying from 0.1 to 0.9, for which experimental data are available [1]. This allowed us to identify also which structural features promote or hinder sodium ions diffusion within solid-state electrolytes, helping the understanding of the composition-structure-conductivity relationship, which is fundamental to efficiently develop new amorphous electrolytes with tailored properties. [1] A. Shastri, D. Watson, Q. Ding, Y. Furukawa, S.W. Martin, Solid State Ionics, 2019, 340, 115013. [2] M. Bertani and A. Pedone, J. Phys. Chem. C, under revision.

Primary author(s) : Dr. BENASSI, Matilde (Università degli Studi di Modena e Reggio Emilia); Dr. BERTANI, Marco (Università degli Studi di Modena e Reggio Emilia); Prof. PEDONE, Alfonso (Università degli Studi di Modena e Reggio Emilia)

Presenter(s) : Dr. BENASSI, Matilde (Università degli Studi di Modena e Reggio Emilia)