
Optimization of composition and interfacial properties of halide solid electrolytes

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Description:

One of the main challenges in the development of all-solid-state batteries is the search for suitable solid electrolytes (SEs) that simultaneously exhibit high ionic conductivity, chemical stability, and compatibility with the electrode materials. The Li_2ZrCl_6 (LZC) SE is a promising candidate due to its high lithium-ion conductivity and excellent (electro)chemical stability. Nevertheless, the practical application of LZC requires improvement of the bulk and interfacial ionic conductivity of the SE. For this purpose, we will calculate reactivity and ionic conductivity using ab initio molecular dynamics simulations of interface models.

Based on the result of these simulations we will propose strategies for the optimization of bulk and interfacial properties of the LZC SE by tuning the electrolyte composition.

Web:

Source

URL:<https://web.computaex.es/en/proyectos/optimization-composition-and-interfacial-properties-halide-solid-electrolytes>