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Transition metal impurities in the solid electrolyte LLZO ($Li_7La_3Zr_2O_{12}$): Transport rates and their impact on Li-ion mobility[1]

SHENG YANG, DONALD SIEGEL, Univ of Michigan - Ann Arbor — LLZO has many properties of an ideal solid electrolyte in lithium-ion batteries since it could enable the use of high voltage electrodes and hence enhance the energy density of lithium ion batteries. With supervalent cation doping such as Al^{3+}, Ga^{3+} on the Li-site, the room temperature ionic conductivity of the cubic LLZO can accomplish high ionic conductivity up to 1mS/cm. However, some experiments suggest that mutual diffusion layers were formed between LLZO and cathode where transition metal (TM) diffused into LLZO, which could possibly lead to large interfacial resistance. In this study, we quantified the performance of LLZO after doping with cobalt, manganese, iron and nickel. In particular, we used molecular dynamics simulations with empirical Morse-type potentials to investigate the TM transport rates and their impact on Li-ion mobility. Our work indicates that TM impurities diffuse slower than Li-ion and they will result in a decrease in the Li-ion mobility by blocking Li-ion pathways. Our work shines light on the origin of interfacial resistance between LLZO and different cathodes.

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