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Density functional and molecular dynamics studies of solid electrolyte $Li_7La_3Zr_2O_{12}$ MICHELLE JOHANNES, KHANG HOANG, NOAM BERNSTEIN, Naval Research Laboratory — Garnet-type structured $Li_7La_3Zr_2O_{12}$(LLZO) is considered as a promising candidate for Li-ion battery solid electrolytes because of its high ionic conductivity and electrochemical and chemical stability. We use first-principles density-functional theory calculations and molecular dynamics simulations to reveal the underlying mechanism that drives a tetragonal to cubic transition at elevated temperatures, and also to explain why the cubic phase can be stabilized with the incorporation of a certain amount of impurities such as Al. We show that the relationship between the observance of a cubic phase and the measurement of a substantially higher ionic conductivity is a secondary effect not directly attributable to the presence of Al in the crystal structure. Suggestions for enhancing the ionic conductivity in LLZO will also be discussed.

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