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Structural phase transition and Li-ion diffusion in $Li_7La_3Zr_2O_{12}$ KHANG HOANG, North Dakota State University, NOAM BERNSTEIN, MICHELLE JOHANNES, Naval Research Laboratory — Garnet-type $Li_7La_3Zr_2O_{12}$ (LLZO) is a promising candidate for solid electrolytes in Li-ion battery applications because of its high ionic conductivity and electrochemical and chemical stability. The material has a low-conductivity tetragonal phase and a high-conductivity cubic phase. It has been reported that the cubic phase can be stabilized at ambient conditions, usually with the incorporation of a certain amount of supervalent impurities. In this talk, we present results from density-functional theory and variable cell shape molecular dynamics simulations, and discuss the origin of structural phase transition, effects of extrinsic impurities, and diffusion of Li ions in LLZO. By identifying relevant mechanisms and critical concentrations of the impurities (Li vacancies) for achieving the high-conductivity phase, this work shows how controlled synthesis could be used to improve the material's electrolytic performance.

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