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LLZO: Al, Ta, Nb, W –different dopants and their effect on microstructure and lithium diffusion

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To understand the impact of different dopants (Al, Ta, Nb, W) on the structure and ion conductivity of the solid electrolyte LLZO (Li7La3Zr2O12) on all length scales, we performed XRD, X-PDF, 6Li NMR and neutron diffraction experiments. The dopants Nb and Ta yielded cubic structured LLZO with highest ionic conductivities amongst this class of solid state electrolytes. Additionally, we observed that mechanical treatment of these materials cause a symmetry reduction : Ia3̄d →I4̄3d and a geometrically frustrated local structure. To understand the impact on the Li ion conductivity, neutron powder diffraction and 6Li-NMR were utilized. To this end, impedance spectroscopic and temperature dependent 6Li NMR measurements are used to determine the Li ion conductivity. Despite the finding that, in some materials, disorder can be beneficial, with respect to ionic conductivity, pulse-field gradient NMR measurements of the long-range transport up to 500 µm indicate a bulk Li+ diffusion barrier in the lower symmetric structure. The geometric frustration and symmetry reduction can be cured and converted back into the higher symmetric garnet structure by temperature treatment. The Li+ conductivity enhancing effect of the temperature treatment is proven by impedance measurements of sintered pellets.

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