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Energy Landscape for Li-Ion Diffusion in the Garnet Type Solid Electrolyte material Li_{6.5}La₃Zr_{1.5}Nb_{0.5}O₁₂ (LLZO-Nb)

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The detailed investigation of innovative solid electrolytes featuring promising properties, such as a high ionic conductivity, that make it suitable for an application in next-generation batteries is one of the key strategies to expand the understanding of corresponding structure-property-relationships which than allows for further tailoring of the materials properties as demanded.

Here, we report on the investigation of the well-known and commercially available material $Li_{6.5}La_3Zr_{1.5}Nb_{0.5}O_{12}$ (LLZO-Nb) by powder X-ray and powder neutron diffraction as well as by temperature-dependent synchrotron powder diffraction experiments. Based on the experimental neutron data the Li-ion diffusion pathways are analyzed applying the maximum entropy method as well as the one-particle potential formalism. The obtained results allow for a visualization of the energy landscape for Li-ion motion within the garnet structure.

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