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The Relationship of Li⁺ Displacement and Temperature in the Garnet Oxides Li_{7-x}La₃Zr_{2-x}Ta_xO₁₂

The lithium containing garnet oxides of Li₇La₃M₂O₁₂ (M = Ta, Nb) were reported to have Li⁺ conducting abilities back in 2003.¹ Since then lithium containing garnet oxides have been identified as a electrolyte candidate for lithium ion batteries as they exhibit the physical and chemical properties desired for a solid-state electrolytes.² The most notable garnet oxide material is the cubic phase (Ia-3d) Li_{6.4}La₃Zr_{1.4}Ta_{0.6}O₁₂ which has a reported Li⁺ conductivity of 1×10^{-3} S cm⁻¹.³ Here the structures and Li⁺ site occupancies of garnet series of Li_{7-x}La₃Zr_{2-x}Ta_xO₁₂ (x = 0, 0.25, 0.50, 0.75, 1.00) was further explored. A one step heating synthesis was employed for garnet preparing. Successful cubic phase garnet synthesis was confirmed with X-ray powder diffraction. Determination of lithium occupancy at the Li24 and Li96 sites was achieved with high-resolution neutron powder diffraction. NPD data were collected at room temperature, 200°C, 400°C and 600°C.

References

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Topic

Advanced Materials

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