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The Relationship of Li+ Displacement and Temperature in the Garnet Oxides Li7-xLa3Zr2-xTaxO12

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) Li6.4La3Zr1.4Ta0.6O12 which has a reported Li+ conductivity of 1 x 10-3 S cm-1.3 Here the structures and Li+ site occupancies of garnet series of Li7-xLa3Zr2-xTaxO12 (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℃, 400℃ and 600℃.

References
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Topic

Advanced Materials

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