Contribution ID: **14** Type: **Poster**

Exploring structure-property relationships in NASICON-type Sn-doped LiTi2(PO4)3

Monday, 11 November 2019 17:00 (1 hour)

NASICON-type materials such as rhombohedral LiTi2(PO4)3 (LTP), belonging to the R-3c space group, have been studied as potential solid-state electrolytes because of their thermal and chemical stability, as well high ionic diffusion attributed to their 3D framework consisting of TiO6 octahedra, corner-linked to PO4 tetrahedra, allowing for fast transportation of Li+ cations. [1] However, the room-temperature conductivity of LTP is not practical for use in Lithium ion batteries (LIBs) as it is approximately 4×10-7 S cm-1. [2] Research around this class of materials has been focused on ways to increase their conductivities, including tuning the bottleneck size by substituting Ti4+ with other cations such as Zr4+ and Hf4+, and increasing Li+ concentration by lattice site substitution with M3+ cations as in Al-doped LTP. [3, 4] In the former case, substitutions in the framework with cations of larger ionic radii increase the lattice constants a and c, resulting in a bigger bottleneck size, thus higher conductivity of the mobile cations, Li+.

In this work, we explore the possibility of lattice substitution as well as investigate if Sn4+-doped LTP formulations exhibit an improved ionic conductivity compared to LTP. Materials of the general formula Li□Ti□_(2-x) □Sn□_x (□PO□_4)_3 (for 0, 2, 4, 6, 8, 10, 50 mole % Sn) have been synthesized following the conventional solid-state method. Room-temperature X-ray diffraction was employed as the primary characterization technique, giving insight into the phase compositions and relative phase purities of the products. Room-temperature Raman spectroscopy was used to further establish the structural properties of LTP as a function of dopant percentage. Information about the phase stabilities of the aforementioned materials was obtained by differential thermal analysis, establishing whether or not there was any temperature-dependent polymorphism exhibited by the said products. The room-temperature conductivities were determined using electrochemical impedance spectroscopy.

References:

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Session Classification: Poster Session 1

Track Classification: Materials