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The enhancement of the ionic conductivity of Sn-doped $\text{LiTi}_2(\text{PO}_4)_3$ by formation of an Al, Sn co-doped system

NASICON-type $\text{LiTi}_2(\text{PO}_4)_3$ (LTP) has been studied as a potential solid-state electrolyte material in Li ion batteries (LIBs), owing to its thermal stability and fast ionic mobility. 1 The structure of LTP consists of TiO_6 octahedra corner-linked to PO_4 tetrahedra, forming a helix about the c-axis. Li can occupy two sites in the structure: the more stable six-fold O coordinated M1 and the eight-fold O coordinated M2, which is less stable. The net ionic movement is described as M1-M2-M1. The 3D network allows for the migration of alkali ions through the structure, making the material a candidate as an electrolyte in LIB. However, its room temperature conductivity in the order of 10^{-7} S/cm is too low for practical applications in LIBs. 1,2 Research around this class of materials has been focused on ways to increase their conductivities, including tuning the bottleneck size by substituting Ti^{4+} with other cations such as Zr^{4+} and Hf^{4+} , and increasing Li^+ concentration by lattice site substitution with M^{3+} 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 Al^{3+} -doped systems, the presence of excess Li^+ required for charge balance, increases the amount of charge carriers.

In this work, we investigate the effect of $\text{Al}^{3+}/\text{Sn}^{4+}$ co-doping at the Ti^{4+} site on the room temperature conductivity of LTP. The structural properties have been studied using synchrotron PXRD and pair distribution function (PDF). Raman spectroscopy provided insight on the changes in local order around the substitution sites as well as confirming the phase composition of the material in question. LATSP showed improved ionic conductivity of 8.04×10^{-6} S/cm.

References

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Summary

Primary author: NKALA, Gugulethu C. (Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg)

Co-authors: Mr MASINA, Sikhumbuzo M. (Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg); Prof. BILLING, Caren (Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg); Dr FORBES, Roy P. (Molecular Sciences Institute, School of Chemistry,

University of the Witwatersrand, Johannesburg); Prof. BILLING, David G. (Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg)

Presenter: NKALA, Gugulethu C. (Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg)