Abstract Submitted
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Design and synthesis of a crystalline LiPON electrolyte[1] N.A.W. HOLZWARTH, KEERTHI SENEVIRATHNE, CYNTHIA S. DAY, ABDESSADEK LACHGAR, Wake Forest U., MICHAEL D. GROSS, Bucknell U. — In the course of a computation study of the broad class of lithium phosphorus oxy-nitride materials of interest for solid electrolyte applications, Du and Holzwarth,[2] recently predicted a stable crystalline material with the stoichiometry Li_2PO_2N. The present paper reports the experimental preparation of the material using high temperature solid state synthesis and reports the results of experimental and calculational characterization studies. The so-named *SD*-Li_2PO_2N crystal structure has the orthorhombic space group $Cmc2_1$ with lattice constants a=9.0692(4) Å, b=5.3999(2) Å, and c=4.6856(2) Å. The structure is similar but not identical to the predicted structure, characterized by parallel arrangements of anionic phosphorus oxy-nitride chains having planar P−N−P−N backbones. Nitrogen 2pπ states contribute to the strong bonding and to the chemical and thermal stablility of the material in air up to 600° C and in vacuum up to 1050° C. The measured Arrhenius activation energy for ionic conductivity is 0.6 eV which is comparable to computed vacancy migration energies in the presence of a significant population of Li^+ ion vacancies.

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[2]Y. A. Du and N. A. W. Holzwarth, *Phys. Rev. B* **81** 184106 (2010)

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