

Abstract Submitted  
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**Prediction of a new crystalline lithium phosphorus oxynitride –  $\text{Li}_2\text{PO}_2\text{N}$** <sup>1</sup> N. A. W. HOLZWARTh, YAOJUN A. DU<sup>2</sup>, Wake Forest University — Lithium phosphorus oxynitride materials have been investigated for many years, especially in relation to the thin film electrolyte LiPON, developed at Oak Ridge National Laboratory.<sup>3</sup> We have carried out first principles simulations of related crystalline materials in an attempt to understand the sources of stability and mechanisms of Li ion conductivity in these materials. Starting with crystalline  $\text{LiPO}_3$  which has twisted phosphate chains,<sup>4</sup> we consider the possibility of modifying the structure by substituting N and Li for O. The optimized structures are computed to have regularized phosphate chains which form planar -P-N-P-N- backbones. To the best of our knowledge, the new predicted crystals, which we call  $s_1\text{-Li}_2\text{PO}_2\text{N}$  with a 24 atom unit cell and  $s_2\text{-Li}_2\text{PO}_2\text{N}$  with a 12 atom unit cell, have not yet been observed experimentally. We suggest several possible exothermic reaction pathways to synthesize these crystals.

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<sup>3</sup>J. B. Bates *et al*, *Solid State Ionics* **53-56** 647-654 (1992).

<sup>4</sup>E. V. Marashova, *Crystallography Reports* **46** 942-946 (2001).

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