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First-principles simulations of extended phosphorus oxynitride structures in LiPON glasses[1] YAOJUN DU, N. A. W. HOLZWARTH, Wake Forest University — The thin film electrolyte LiPON, having the composition of $Li_{3+x}PO_{4-y}N_z$ with $x = 3z - 2y$, was developed at Oak Ridge National Lab in the 1990's for use in solid state batteries and related applications.[2] In an effort to understand and to optimize properties of this electrolyte material, we expanded previous studies of isolated defects in crystalline Li_3PO_4[3] to focus on more complicated phosphate structures based on combinations of tetrahedral P−O bonds and bridging P−O−P bonds. For example, crystalline $LiPO_3$[4] and P_2O_5[5] are composed of phosphate structures with linear and branched chains, respectively. Both these and related structures derived from substituting O with N and adjusting mobile Li ion concentrations approximate components found in LiPON films.[2] In the simulated structures, we find that N is energetically more stable at bridging bond sites than at tetrahedral sites by 2-3 eV and that the Li ion migration energies are 0.5−0.6 eV, similar to values measured in LiPON films.

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