Li$_{14}$(PON$_3$)$_2$O: Computational study of a possible new electrolyte for Li ion batteries

AHMAD AL-QAWASMEH, N. A. W. HOLZWARTH, Wake Forest Univ — Recently, Li$_{14}$(PON$_3$)$_2$O, containing Li$_6$PON$_3$ and Li$_2$O groups within a trigonal crystal structure (space group $P\overline{3}$ (#147)) has been synthesized by Baumann and Schnick. We report the results of a first principles computational study of this material in comparison with other crystalline electrolytes having LiPON composition and isolated tetrahedral oxonitridophosphate ions such as Li$_3$PO$_4$ and Li$_7$PN$_4$. The structure of Li$_{14}$(PON$_3$)$_2$O is characterized by a relatively large Li ion density (0.07 Li/Å$^3$) which is between that of Li$_3$PO$_4$ (0.04 Li/Å$^3$) and Li$_2$O (0.09 Li/Å$^3$). Using a nudged elastic band approach, we find Li ion migration barriers in Li$_{14}$(PON$_3$)$_2$O to be comparable or lower than those of Li$_3$PO$_4$ and Li$_7$PN$_4$. The most efficient migration appears to occur via a vacancy mechanism with net motion within planes perpendicular to the c-axis in the vicinity of the O sites. Models of interfaces of Li$_{14}$(PON$_3$)$_2$O with Li metal were also studied.

1Supported by NSF grant DMR-1507942 and WFU’s DEAC cluster.