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First principles investigation of the superionic electrolyte $\mathbf{Li_7P_3S_{11}}$[1] NICHOLAS LEPLEY, N.A.W. HOLZWARTH, Wake Forest University — $Li_7P_3S_{11}$ has been shown to be a promising superionic conductor for solid state rechargeable batteries with a room temperature conductivity as high as 10^{-3} S/cm and a thermal activation energy as small as E_A=0.12 eV.[2] We have performed first principles modeling studies[3] on this material in order to explain its stability and Li ion migration properties. Our investigation considers optimized crystal structures, migration involving both vacancy and interstitial mechanisms, as well as related materials. We find optimized crystal structures in reasonable agreement with experiment,[4] and the lowest calculated activation energy barrier was found to be E_A=0.15 eV in good agreement with the experimental value.

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[2]F. Mizuno et al., *Solid State Ionics* **177**, 2721 (2006).
[3]N. A. W. Holzwarth, N. D. Lepley, Y. A. Du, *J. Power Sources* **196**, 6870 (2011).
[4]H. Yamane et al., *Solid State Ionics* **178**, 1162 (2007); Y. Onodera et al., *J. Phys. Soc. Jpn.* **79**, 87 (2010), suppl. A.

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