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Investigation of the structural properties of $Na_4P_2S_6$ and $Li_4P_2S_4$[1]

LARRY E. RUSH JR., N.A.W. HOLZWARTH, Wake Forest University — Li-ion batteries were proposed in the 1970's and are currently commercially produced globally for many technological purposes; however, recent studies have suggested that Na-ion conducting materials might be a feasible alternative that could have some advantages over Li-ion batteries. First principles simulations are used in this investigation to examine the structural and physical properties of $Na_4P_2S_6$, a Na-ion conductor, in comparison with its Li-ion conducting analog, $Li_4P_2S_4$. Four model structures are considered including the $C2/m$ ˜structure recently reported by Kuhn and co-workers from their analysis of single crystals of $Na_4P_2S_6$ (ZAAC, 640(5):689-692, April 2014), and three structures related to the $P6_3/mcm$ structure with P site disorder found in 1982 by Mercier and co-workers from their analysis of single crystals of $Li_4P_2S_4$ (JSSC, 43(2):151-162, July 1982). The computational results indicate that both $Na_4P_2S_6$ and $Li_4P_2S_4$ have the same disordered ground state structures consistent with the $P6_3/mcm$ space group, while the optimized $C2/m$structures are meta-stable by 0.1 eV and 0.4 eV per formula unit for $Na_4P_2S_6$ and $Li_4P_2S_4$, respectively.

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