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First Principles Investigation of the Geometrical and Electrochemical Properties of $Na_4P_2S_6$ and $Li_4P_2S_6$.[1] LARRY E. RUSH JR., N.A.W. HOLZWARTH, Wake Forest University — First principles simulations are used to examine the structural and physical properties of $Na_4P_2S_6$ in comparison with its $Li_4P_2S_6$ analog. Four model structures are considered including the $C2/m$ structure recently reported by Kuhn and co-workers[2] from their analysis of single crystals of $Na_4P_2S_6$, and three structures related to the $P6_3/mcm$ structure with P site disorder found in 1982 by Mercier and co-workers[3] from their analysis of single crystals of $Li_4P_2S_6$. The computational results indicate that both $Na_4P_2S_6$ and $Li_4P_2S_6$ have the same disordered ground state structures consistent with the $P6_3/mcm$ space group, while the optimized $C2/m$ structures have higher energies by 0.1 eV and 0.4 eV per formula unit for $Na_4P_2S_6$ and $Li_4P_2S_6$, respectively. Simulations of ion migration suggest that $Na_4P_2S_6$ may have more favorable ionic conductivity compared to $Li_4P_2S_6$.

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[2]ZAAC **640**(5):689-692 (2014)
[3]JSSC **43**:151-162 (1982)

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