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Computational modeling of the structure and the ionic conductivity of the solid electrolyte materials Li_3AsS_4 and its Ge substitutions[1]
AHMAD AL-QAWASMEH, N. A. W. HOLZWARTH, Wake Forest University — Oak Ridge National Laboratory (G. Sahu et al.)[2] reported that the substitution of Ge into Li_3AsS_4 leads to the composition $Li_{3.334}Ge_{0.334}As_{0.666}S_4$ with impressively high ionic conductivity . We use ab initio calculations to examine the structural relationships and the ionic conductivity mechanisms for pure Li_3AsS_4, $Li_{3.334}Ge_{0.334}As_{0.666}S_4$, and other compositions of these electrolytes.

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[2]J. Matter. Chem. A. 2014, **2**, 10396

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