First Principles Computer Simulations of $Li_{10}GeP_2S_{12}$ and Related Lithium Superionic Conductors

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A recent paper by Kamaya *et al.* [1] reported a new crystalline superionic conductor having a compact tetrahedral structure and a stoichiometry of $Li_{10}GeP_2S_{12}$. The room temperature conductivity was reported to be 0.01 S/cm, comparable to liquid electrolyte conductivies and five times higher the compositionally related thio-LISICON material $Li_{3.25}Ge_{0.25}P_{0.75}S_4$ developed earlier [2]. This poster presents a progress report on our work to perform first principles computer simulations for these materials, focussing on the structural, stability, and Li ion mobility properties of idealized crystalline models. From the perspective of our previous studies of Li ion conductivity in lithium thiophosphate electrolytes [3, 4], the effects of introducing Ge can be assessed.

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[1] N. Kamaya *et al.*, Nature Materials **10**, 682 (2011).

[2] R. Kanno *et al.*, J. Electrochem. Soc. **148**, A742 (2001).

[3] N. A. W. Holzwarth *et al.*, J. Power Sources **196**, 6870 (2011).

[4] N. D. Lepley *et al.*, J. Electrochem. Soc. **159**, A538 (2012).

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