SIMULATIONS OF IDEALIZED SOLID ELECTROLYTES*

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Pioneering work at Oak Ridge National Laboratory has shown that solid electrolytes are an important component of advanced battery technology. Inspired by that work and by other experimental efforts, we have performed computer simulations of crystalline electrolytes such as lithium phosphates, lithium phosphorous oxy-nitrides, and lithium thiophosphates and some related sodium electrolytes in order to gain insight into the structural and ion mobility properties of these technological candidates. In addition to simulations of the bulk materials, simulations of interfaces of these electrolytes with lithium or sodium metal anodes show promising results in terms of improving the stability of battery technology.

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