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First-Principles Molecular Dynamics Simulations of Liquid $Li_4BN_3H_{10}$:Structural Characterization and Dynamics of Hydrogen Release DAVID FARRELL, CHRISTOPHER WOLVERTON, Northwestern University, Department of Materials Science and Engineering — The recently discovered $Li_4BN_3H_{10}$ compound is a promising hydrogen storage material due to its high capacity for hydrogen desorption (>10 wt.%) and favorable thermodynamics for low-temperature H_2 release. However, elevated temperatures are necessary for appreciable H_2 desorption, pointing to kinetic limitations. Further, $Li_4BN_3H_{10}$ is liquid at these H_2 release temperatures. In an effort to characterize the liquid structure and uncover the atomistic mechanisms for H_2 release, we have performed first-principles molecular dynamics simulations of liquid $Li_4BN_3H_{10}$. Our calculations give the temperature-dependent liquid structure, which we compare in detail with that of the crystalline solid. We are also able to ascertain the latent heat of melting, an important contribution to understanding the thermodynamics of H_2 release from this material. Finally, we present preliminary work on the atomistic mechanisms of hydrogen desorption from the liquid based on temperature accelerated molecular dynamics.

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