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**First-Principles Study of Native Defects in $Li_4BN_3H_{10}$ Under Varied Chemical Conditions** DAVID FARRELL, CHRISTOPHER WOLVERTON, Northwestern University — Hydrogen desorption from many complex hydrides, such as $Li_4BN_3H_{10}$, is known to be kinetically limited. At temperatures below melting, the motion of point defects is one possible factor affecting chemical reactions. Therefore, an understanding of their formation and migration will yield insight into the kinetic limitation of hydrogen desorption. To explore this, we have determined the 0 K formation energy for a number of neutral and charged point defects in $Li_4BN_3H_{10}$ under a variety of chemical conditions via density functional theory calculations. We determined chemical potentials based on thermodynamically predicted hydrogen desorption reactions and provide a physical interpretation of the resulting equilibrium conditions. Our results indicate that: 1) The lowest energy defect varies with chemical conditions. 2) neutral defects are always lower energy than analogous pairs of oppositely charged defects. 3) Hydrogen defects are rarely the lowest energy defect.

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