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First-Principles Calculations of van't Hoff Plots for Novel Hydrogen-Storage Materials[1] NIKOLAI ZARKEVICH, D.D. JOHNSON, Department of Materials Science and Engineering, and Materials Computation Center, University of Illinois at Urbana-Champaign — A van't Hoff plot, log(P) vs. 1/T, provides information on the free-energy change in a reaction and is widely used to characterize hydrogen-storage materials. Recently, a new reaction of $LiBH_4$ destabilized by MgH_2 (yielding over 11 wt.% of H_2) was proposed.[2] Here we investigate this reaction and its products by first-principles calculations and construct the van't Hoff plot for a direct comparison to experiment. Although it is often assumed that there is a constant slope in the van't Hoff plot for ease of interpretation, we find an important non-linearity arising from temperature-dependent vibrational entropy difference, etc. This non-linearity can be critical for an accurate comparison to experimental data, and between various reactions to determine optimal hydrogen-storage systems. Including these effects, we find agreement with recent measurements.

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[2]J.J. Vajo et al., J. of Phys. Chem. B 109, p.3719 (2005)

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