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**The Importance of van der Waals Interactions in the Stability of the Phases of $Mg(BH_4)_2$** BRIAN KOLB, Wake Forest University, ANDRZEJ BIL, ALEKSEY KOLMOGOROV, University of Oxford, TIMO THONHAUSER, Wake Forest University — As hydrogen gains attention as a potential replacement for fossil fuels, materials to store hydrogen safely and efficiently are becoming increasingly important. Metal borohydrides are attracting much attention for this role and, in particular, $Mg(BH_4)_2$ is a promising candidate for hydrogen storage because of its relatively high hydrogen content (over 12 wt%) and the abundance of its constituent elements. This system has been investigated previously, both experimentally and via density functional theory (DFT) studies. These two approaches give conflicting results, however, regarding the identity of the low-temperature ground-state. In this work, we investigate the impact of van der Waals (vdW) interactions on the stability of various phases of $Mg(BH_4)_2$. vdW interactions are included both through the fully self-consistent vdW-DF approach as well as the semi-empical PBE-D/PBE-D* approach. Our results settle the longstanding discrepancy between theory and experiment, as we find inclusion of vdW interactions stabilizes the experimentally determined ground-state structure at low temperature, relative to those predicted by previous DFT studies.

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