

Van der Waals interactions in the ground state of $\text{Mg}(\text{BH}_4)_2$ from density functional theory.

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To resolve an outstanding discrepancy between experiment and theory regarding the ground-state structure of $\text{Mg}(\text{BH}_4)_2$, we examine the importance of long-range dispersive interactions on the compound's thermodynamic stability. Careful treatment of the correlation effects within a recently developed nonlocal van der Waals density functional (vdW-DF) leads to a good agreement with experiment, favoring the α - $\text{Mg}(\text{BH}_4)_2$ phase (P6122) and a closely related Mn(BH_4)₂-prototype phase (P3112) over a large set of polymorphs at low temperatures. Our study demonstrates the need to go beyond (semi)local density functional approximations for a reliable description of crystalline high-valent metal borohydrides.

Adres publiczny

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