

Abstract Submitted
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Atomic and electronic structure of alkali borohydrides: An *ab initio* study W. GEMPEL, N. KIOUSSIS¹, Department of Physics, California State University Northridge, D. PAPACONSTANTOPOULOS, Center for Computational Materials Science, Naval Research Laboratory — Alkali borohydrides MBH₄ (M = Na, K) have attracted great interest recently due to their potential applications as hydrogen storage materials and energy carriers for fuel cells due to the extremely large gravimetric capacity. At low temperature the compounds crystallize with a tetragonal structure having P42/nmc symmetry in which the [BH₄]⁻ complexes are ordered. We have carried out total-energy *ab initio* electronic structure calculations based on the Projector Augmented Wave (PAW) method to calculate the atomic and electronic structure of this series. The lattice constants and various bond lengths are in good agreement with experiment. Results of the trend of the heat of formation for the hydriding/dehydriding reactions, the band structure, the density of states, and bonding properties of the [BH₄]⁻ complexes will be discussed.

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