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Electronic Structure and Molecular Dynamics Calculations for KBH_4[1] DIMITRIOS PAPACONSTANTOPOULOS, ANDREW SHABAEV, KHANG HOANG, George Mason University, MICHAEL MEHL, Naval Research Laboratory, NICHOLAS KIOUSSIS, UC at Northridge — In the search for hydrogen storage materials, alkali borohydrides MBH_4 (M=Li, Na, K) are especially interesting because of their light weight and the high number of hydrogen atoms per metal atom. Electronic structure calculations can give insights into the properties of these complex hydrides and provide understanding of the structural properties and of the bonding of hydrogen. We have performed first-principles density-functional theory (DFT) and tight-binding (TB) calculations for KBH_4 in both the high temperature (HT) and low temperature (LT) phases to understand its electronic and structural properties. Our DFT calculations were carried out using the VASP code. The results were then used as a database to develop a tight-binding Hamiltonian using the NRL-TB method. This approach allowed for computationally efficient calculations of phonon frequencies and elastic constants using the static module of the NRL-TB, and also using the molecular dynamics module to calculate mean-square displacements and formation energies of hydrogen vacancies.

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Dimitrios Papaconstantopoulos
George Mason University

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