Structural, electronic, elastic and thermodynamical properties of BaSrLiH$_3$

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1. Introduction – In this paper, we aim to study the structural, electronic, elastic and thermodynamical properties of BaSrLiH$_3$ using ab initio calculations within the generalized gradient approximation and local density approximation. In particular, the lattice constant, bulk modulus, second-order elastic constants (C$_{ij}$) and electronic band structures are calculated and compared with the available experimental and other theoretical values. In addition, we have also predicted the variation of Young’s modulus (E), Poisson’s ratio (v), sound velocities, Debye temperature and melting temperature (Tm) as a function of the Ba concentration (x).

2. Computational method - The calculations were performed within GGA and LDA for density functional theory (DFT), using the PP-PW method as implemented in the ABINIT computer code (http://www.abinit.org). The ABINIT code is a common project of the Catholic University of Louvain, Corning Inc. and other contributors. Only the outermost electrons of each atom were explicitly considered in the calculation. The effect of the inner electrons and the nucleus (the frozen core) was described within a pseudopotential scheme.

3. Results and Discussion - The perovskites BaSrLiH$_3$ have ideal cubic structure (SG: Pm$_3$m), where the atomic positions in the elementary cell are Ba/Sr: (1/2, 1/2, 1/2), Li: (0, 0, 0) and H: (1/2, 0, 0). The calculated lattice parameters, bulk modulus and pressure derivative of BaSrLiH$_3$ within GGA and LDA, using the PP-PW method, are summarized in table 1, along with the available experimental data.

Tabla I. Calculated lattice parameter a, bulk modulus B$_0$ and its pressure derivative B’ for BaSrLiH$_3$ alloys at equilibrium volume compared to experiment and other theoretical calculations.