ENTHALPIES OF FORMATION OF TRANSITION METAL AND RARE-EARTH BORIDES. A FIRST PRINCIPLES STUDY.

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Calculations based on the density functional theory have achieved considerable reliability for the prediction of the properties of materials. In the present work, we have studied the structural stability of binary intermetallic compounds of boron with transition metals and rare-earth elements. The density functional (DFT) calculations have been performed with the Vienna *ab initio* simulation package (VASP) [1], making use of the projector augmented waves (PAW) technique [2, 3]. For the generalized gradient approximation (GGA) exchange correlation functional, we have used the Perdew-Burke-Ernzerhof parameterization (PBE) [4].

The calculated values of the lattice parameters at $T = 0$ K of the stable compounds agree well with the experimental values [5]. The calculated enthalpies of formation of these compounds are compared to the values obtained with calorimetric methods [6, 7]. In the whole, the calculated values of the formation enthalpies of formation the borides in their ground state are in good agreement with the experimental ones when available. The calculated values have also been compared with those previously published in various publications or data bases. Finally, the evolution of the enthalpies of formation of the borides along the 3d, 4d, and 5d series of the transition metals and the series of rare-earth Sc, Y, La and La to Gd to Lu is discussed.

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