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THEORY STUDY OF STRUCTURAL, ELECTRONIC AND THERMAL PROPERTIES OF TERNARY LANTHANIDE HYDRIDE CsCaH3.

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Abstract

Perovskite hydrides ABH3 are gaining much interest for the use as potential hydrogen storage because of their cubic structure and their light weight (CsCaH3, RbCaH3, BaLiH3 and SrLiH3). However, most of these materials are not well-described and thermodynamic data are absent. First-principles calculations offer one of the most powerful tools for carrying out theoretical studies of an important number of physical chemical properties with great accuracy.

The structural, electronic and thermal properties of the ternary lanthanide hydride CsCaH3 are investigated using the full potential linearized augmented plane wave method (FP-LAPW). The calculations are performed using the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange-correlation potential [1]. The contribution of the different bands was analysed from total and partial density of states curves.

The thermal effect on the lattice constant, bulk modulus, Debye temperature and heat capacity Cv was predicted using the quasi harmonic Debye model (figure 1 and 2). These results were in favourable agreement with previous theoretical works and the existing experimental data [2]. The theoretical investigations of the electronic and thermal properties of CsCaH3 are necessary for more technological applications.The perovskite hydride CsCaH3 is interesting for the use as potential hydrogen storage material because of his light weight, low cost and high capacitie of hydrogen.

Key words: *DFT, FP-LAPW,Dos, perovskite, hydride*

References

[1] T. Jaron, W. Grochala and R. Hoffmann, J. Materials Chemistry, 2006, **16**, 1154-1160.

[2] F. Gingl, T. Vogt, E. Akiba and K. Yvon, JAlloys Compd, 1999, **282**, 125-129 .

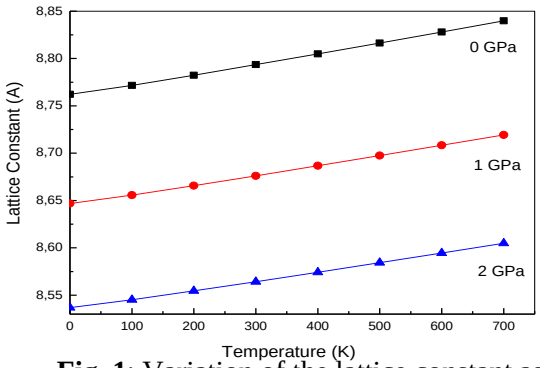

Fig. 1: Variation of the lattice constant as a function of temperature at pressures of 0, 1 and 2 GPa for CsCaH3.

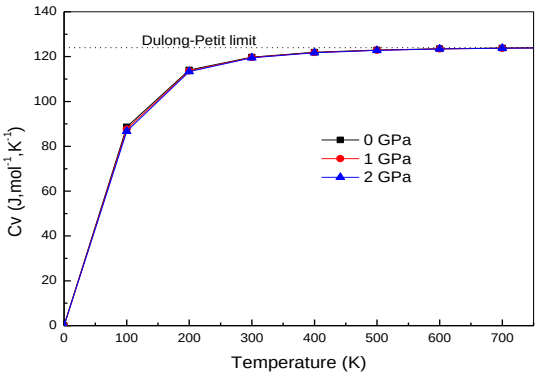

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Fig. 2: Variation of the heat capacities C_V as a function of temperature at pressures of 0, 1 and 2 GPa for CsCaH3.