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First-Principles Study of the Jahn-Teller Distortion in the $Ti_{1-X}V_XH_2$ and $Zr_{1-X}Nb_xH_2$ Alloys RAMIRO QUIJANO, ROMEO DE COSS, CINVESTAV-Unidad Merida, DAVID SINGH, Oak Ridge National Laboratory, USA — The transition metal dihydrides TiH_2 and ZrH_2 present the fluorite structure (CaF_2) at high temperature but undergoes a tetragonal distortion with c/a<1 at low temperature. Electronic band structure calculations have shown that TiH_2 and ZrH_2 in the cubic phase display a very flat band at the Fermi level. Thus the low temperature tetragonal distortion has been associated to a Jahn-Teller effect. In order to understand the role of band filling in controlling the structural instability of the transition metal dihydrides, we have performed a first-principles total energy study of the $Ti_{1-X}V_xH_2$ and $Zr_{1-x}Nb_xH_2$ alloys. The calculations were performed using FP-LAPW method within the (DFT) and we use the GGA for exchange correlation functional energy. The critical concentration for which the Jahn-Teller effect is suppressed, was determined from the evolution of the tetragonal-cubic energy barrier. We discuss the electronic mechanism of the structural-instability, in terms of the band filling. From the obtained results we conclude that the tetragonal distortion in TiH_2 and ZrH_2 is not produced only by a Jahn-Teller Effect. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

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