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First-principles study of the Jahn-Teller distortion in transition metal dihydrides.[1] RAMIRO QUIJANO, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Mérida, México — 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. Early 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. Previous total energy calculations of the tetragonal distortion for TiH_2 within the Density Functional Theory (DFT), find that the ground state correspond to a tetragonal structure with c/a>1, in contradiction with the experimental observation (c/a<1). In the present work, we have performed full-potential LAPW calculations using the Local Density Approximation (LDA) and the Generalized Gradient Approximation (GGA) for the exchange correlation functional energy. Special attention was paid to the convergence of the total-energy calculations, since in TiH_2 the energy differences for a tetragonal distortion at constant volume are only fractions of 1 mRy. We find that the ground state of TiH_2 and ZrH_2 corresponds to a tetragonal distorted fluorite structure with c/a<1, in agreement with the experimental observations. The same behavior is predicted for HfH_2. The electronic band structure of the three systems is analyzed in the context of the Jahn-Teller effect.

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