

Abstract Submitted
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Effect of pressure on the tetragonal distortion in TiH₂: a first-principles study R. DE COSS, R. QUIJANO, Department of Applied Physics, Cinvestav-Merida, A.P. 73 Cordemex 97310 Merida, Yucatan, Mexico, D.J. SINGH, Oak Ridge National Laboratory, USA — The transition metal dihydride TiH₂ present the fluorite structure (CaF₂) at high temperature but undergoes a tetragonal distortion with $c/a < 1$ at low temperature. Early electronic band structure calculations have shown that TiH₂ in the cubic phase display a nearly flat double degenerated band at the Fermi level. Thus the low temperature tetragonal distortion has been associated to a Jahn-Teller effect. Nevertheless, recently we have show that the instability of fcc-TiH₂ is likely to be related with a van Hove singularity. In the present work, we have performed *ab-initio* calculations of the electronic structure and the tetragonal distortion for TiH₂ under pressure (0-30 GPa). We found that the fcc-fct energy barrier and the tetragonal distortion increases with pressure. The evolution of the tetragonal distortion is analyzed in terms of the electronic band structure. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 49985.

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