

## Accepted Manuscript

The effect of relaxation on the structural and electronic properties of a terbium superstoichiometric dihydride

Zahia Ayat , Aomar Boukraa , Bahmed Daoudi ,  
Abdelouahab Ouahab

PII: S0577-9073(17)30278-2  
DOI: [10.1016/j.cjph.2017.06.017](https://doi.org/10.1016/j.cjph.2017.06.017)  
Reference: CJPH 330



To appear in: *Chinese Journal of Physics*

Received date: 16 March 2017  
Revised date: 3 June 2017  
Accepted date: 29 June 2017

Please cite this article as: Zahia Ayat , Aomar Boukraa , Bahmed Daoudi , Abdelouahab Ouahab , The effect of relaxation on the structural and electronic properties of a terbium superstoichiometric dihydride, *Chinese Journal of Physics* (2017), doi: [10.1016/j.cjph.2017.06.017](https://doi.org/10.1016/j.cjph.2017.06.017)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

---

## Highlights

- This is the first time to study the superstoichiometric  $\text{TbH}_{2.25}$  dihydride with  $Pm\bar{3}m$  space group.
- The equilibrium properties (lattice parameter, bulk modulus and its pressure derivative) are determined.
- The partial and total density of states, energy band structure, and valence electron-charge density contours are plotted.

Download English Version:

<https://daneshyari.com/en/article/5488126>

Download Persian Version:

<https://daneshyari.com/article/5488126>

[Daneshyari.com](https://daneshyari.com)