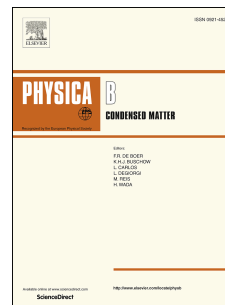


# Accepted Manuscript

First-principles study of structural, elastic, and electronic properties of triclinic TATB under different pressures

Han Qin, Bao-Luo Yan, Mi Zhong, Cheng-Lu Jiang, Fu-Sheng Liu, Bin Tang, Qi-Jun Liu



PII: S0921-4526(18)30621-5

DOI: [10.1016/j.physb.2018.10.003](https://doi.org/10.1016/j.physb.2018.10.003)

Reference: PHYSB 311088

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 22 August 2018

Revised Date: 29 September 2018

Accepted Date: 1 October 2018

Please cite this article as: H. Qin, B.-L. Yan, M. Zhong, C.-L. Jiang, F.-S. Liu, B. Tang, Q.-J. Liu, First-principles study of structural, elastic, and electronic properties of triclinic TATB under different pressures, *Physica B: Physics of Condensed Matter* (2018), doi: <https://doi.org/10.1016/j.physb.2018.10.003>.

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.

First-principles study of structural, elastic, and electronic properties of  
triclinic TATB under different pressures

Han Qin<sup>a,b, \*\*</sup>, Bao-Luo Yan<sup>a,b</sup>, Mi Zhong<sup>a,b</sup>, Cheng-Lu Jiang<sup>a,b</sup>, Fu-Sheng Liu<sup>a,b</sup>,

Bin Tang<sup>c</sup>, Qi-Jun Liu<sup>\* a,b</sup>

<sup>a</sup> School of Physical Science and Technology, Southwest Jiaotong University, Key  
Laboratory of Advanced Technologies of Materials, Ministry of Education of China,  
Chengdu 610031, People's Republic of China

<sup>b</sup> Bond and Band Engineering Group, Sichuan Provincial Key Laboratory (for  
Universities) of High Pressure Science and Technology, Southwest Jiaotong  
University, Chengdu 610031, People's Republic of China

<sup>c</sup> State Key Laboratory of Solidification Processing, Northwestern Polytechnical  
University, Xi'an 710072, People's Republic of China

Correspondence about the paper at the following address and e-mail address:

Han Qin

School of Physical Science and Technology, Southwest Jiaotong University, Chengdu,  
Sichuan 610031, People's Republic of China

E-mail: hanqin1108@163.com

Qi-Jun Liu

School of Physical Science and Technology, Southwest Jiaotong University, Chengdu,  
Sichuan 610031, People's Republic of China

E-mail: qijunliu@home.swjtu.edu.cn

---

\*\* Corresponding author. E-mail: hanqin1108@163.com

\* Corresponding author. E-mail: qijunliu@home.swjtu.edu.cn

Download English Version:

<https://daneshyari.com/en/article/11019654>

Download Persian Version:

<https://daneshyari.com/article/11019654>

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