Ab Initio Calculations of the Structural and Electronics Properties of DoubleTungstates $NaY(WO_4)_2$

Hanane Arioumlil[1*], Faiza Bouamra[1] and Michel Rérat[2]

[1]Department of physic, LASICOM Laboratory, University of Blida 1, Algeria

[2]E2S UPPA, CNRS, IPREM, Université de Pau et des Pays de l'Adour, France

*Corresponding author

ABSTRACT

The tetragonal crystal structure of double tungstates $NaY(WO_4)_2$ has been determined. Our calculations confirm the insulating character of $NaY(WO_4)_2$, the obtained resultswere justified and discussed from the diagrams of bandstructures and density of states DOS and LDOS.

Introduction

Bi-tungstate materials of the general formula $MT(WO_4)_2$, where M is a monovalent alkali cation and T is a trivalent cation, the majority of these crystals have tetragonal symmetry with a random distribution of monovalent and trivalent ions[1] and they have attracted a lot of attention because of their excellent chemical stability in air and also inthe field of spectroscopy specifically for the Laser. In the literature, a few theoretical researches work on double tungstates $NaY(WO_4)_2$ has been determined. The aim of this investigation, is to determine theoretically structural and electronics properties of double tungstates $NaY(WO_4)_2$.

Theoretical Study

The Bi-tungstate $NaY(WO_4)_2$ in his tetragonal phase, ischaracterized by space group I41/a=C^6 with lattice parameters a=b=5.24Å, c=11.38Å and α=β=γ=90°. W occupies the tetrahedral sites composed by the O atoms, Na and Y cations have the same occupancy factors. An ab initio SCF-LCAO-B3LYP calculations are performed with Crystal17 program[3] to determine structural and electronics properties of $NaY(WO_4)_2$.

Results and Discussion

Figure 1, show the primitive NYW cell. The W^{6+} ion iscoordinated by four O^{2-} at a tetrahedral site, representations are performed with J-ice visualization program[4].

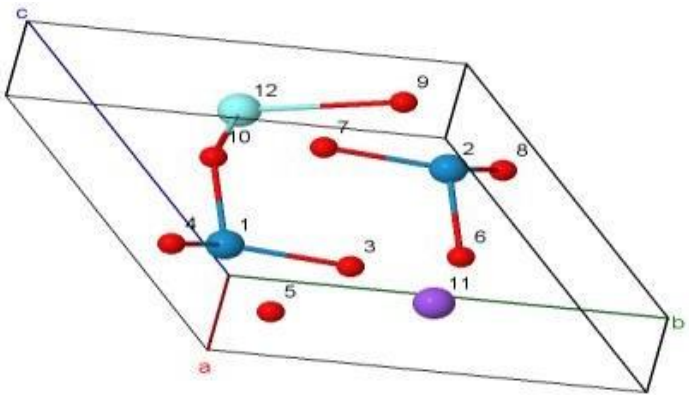

Fig.1. Elementary unit cell of NaY $(WO_4)_2$.

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5

The band structure of $NaY(WO_4)_2$ along the high symmetry points of the irreducible Brillouin zone is shown in Figure2a.Value of the band gap is the difference between the CBM and the VBM equal to 5.48eV, which confirm the insulatorcharacter of $NaY(WO_4)_2$, is in good agreement with experimental results. Total density of states (DOS) and the projected on layer (LDOS) are shown in figure2.b.

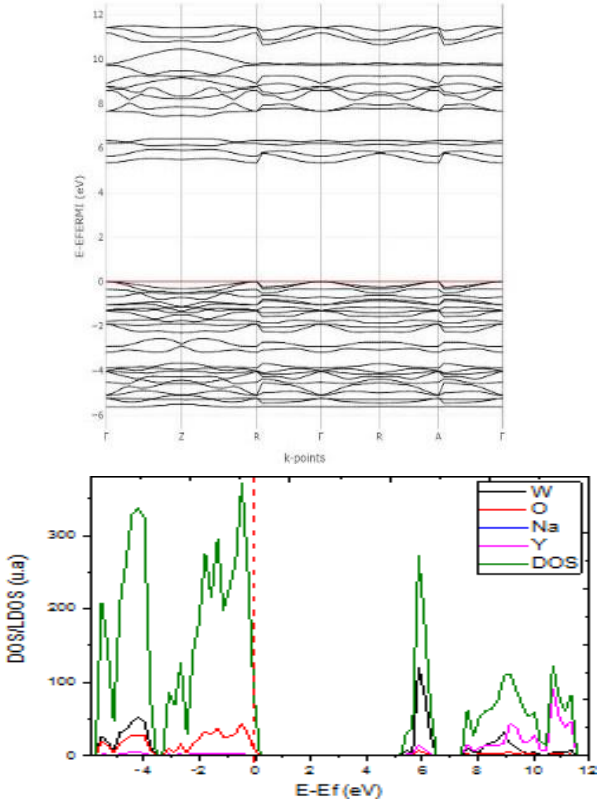

Fig.2. (a) Band structure of NaY $(WO_4)_2$, (b) DOS/LDOS

Conclusion

Double tungstates $NaY(WO_4)_2$ in his tetragonal phase hasbeen studied at the level of SCF-LCAO-B3LYP theory. Calculations shows that is an insulator Materials with calculated band gap of 5.48eV.

Acknowledgments

The authors gratefully acknowledge Chemical-Physicsgroup of IPREM of Pau University.

References

[1] L. Macalik, J. Hanuza, A.A. Kaminskii « Polarized Ramanspectra of the oriented NaY (WO4)2 and KY(WO4)2 single crystals» (2000) 289–297.

[2] HE Yizong, WANG Guofu, HUANC Xiaoying, Luo Zundu, «The Emission and Structure of a New Laser Crystal Nd3 + : NaY(WO4)2»1994,267-271.

[3] R. Dovesi et al., "User's Manual of CRYSTAL17", codeavailable from http://www.crystal.unito.it

[4] *J-ICE: a new Jmol interface for handling and visualizing Crystallographic and Electronics properties*, P. Canepa, R. M. Hanson, P. Ugliengo, M. Alfredsson *J. Appl. Cryst.* 44,225 (2011)

ISBN: 978-81-954993-3-5
DOI: 10.21467/abstracts.122
Series: AIJR Abstracts