Electronic and structural properties of B phase of Nb_2O_5 bulk – A DFT study

Mirele Bastos Pinto (PG), Hélio A. Duarte (PQ) and Heitor A. De Abreu (PQ).

Universidade Federal de Minas Gerais, Departamento de Química – GPQIT, Belo Horizonte Brazil. e-mail: mirele.quimica@gmail.com

Keywords: Niobium pentoxide, DFT, Plane Waves, QTAIM.

INTRODUCTION

The niobium chemistry is still not well understood, nevertheless niobium compounds have attracted interest in many areas due to its strong surface acidity and stability in aqueous medium for various acid-catalyzed reactions. There are several crystallographic phase of Nb_2O_5 that depends on the temperature and pressure to which the materials are submitted. It has been shown that the B phase (B-Nb_2O_5) can be stabilized at room temperature and pressure[1]. This phase is monoclinic and has 28 atom/cell[2]. The understanding of the electronic and structural properties of the bulk and surfaces of Nb_2O_5 is the first step for understanding the catalytic properties of these material at a molecular level. Therefore, the aim of this work is the elucidation of the nature of the chemical bonding and the structural and electronic properties of the B-Nb_2O_5 bulk.

METHODS

All the calculations have been performed through Density Functional Theory (DFT)/plane waves methodology with periodic boundary conditions as implemented in the *Quantum-ESPRESSO package—PWscf*. PBE exchange–correlation (xc) functional with core electrons described by ultrasoft pseudo-potentials were used. A cutoff energy of 60 Ry and charge density cutoff of 400 Ry were used. The k-points density 4x4x4 integrals by Monkhorst and Pack was applied.

RESULTS AND DISCUSSION

The band structure was calculated indicating indirect band gap of 2.6 eV. The experimental gap of this phase is not reported in the literature. For crystalline H-Nb_2O_5 and T- Nb_2O_5 the measured gap was 3.4 eV[3]. Figure 1 shows the total and site-projected DOS calculated for B-Nb_2O_5. The oxygen atom is the one that most contributes to the states around the Fermi level in the valence band. On the other hand, niobium (*d* orbitals) are the largest contributor to the conduction band. This agrees to the Quantum Theory of Atoms in Molecules (QTAIM) atomic charge analysis which are shown in Table 1. The estimated positive atomic charge for Nb is reasonable since oxygen atom is more electronegative (χ). The QTAIM topological analysis and ELF indicate ionic character for Nb–O bond.

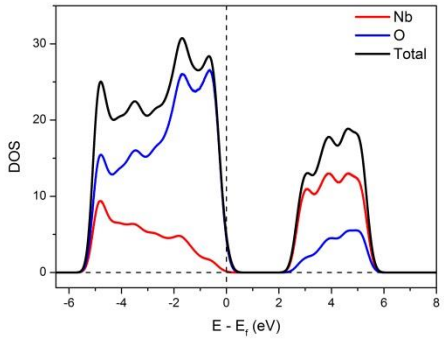

Figure 1. Total and projected DOS over the atoms of Nb_2O_5.

Table 1. Atomic charges in QTAIM analysis. Volume ($Borh^3$) is the volume of the basins occupied by the atoms.

Atoms	Charge	Volume ($Borh^3$)	χ
O1	-1.07	98.63	3.44
O2	-1.01	92.83	
O3	-1.16	81.51	
Nb	2.72	67.10	1.60
Total		2358.02	

CONCLUSIONS

Structural and electronic calculated properties for the crystalline B phase of Nb_2O_5 bulk are in good agreement with the experimental data. Preliminary results point out the niobium sites as the most acidic, which will be important for the chemical reactivity of the surfaces.

ACKNOWLEDGMENTS

INCT-acqua, FAPEMIG, CAPES and CNPq.

[1] I. Nowak and M. Ziolek, Chemical Reviews **99**, 3603-3624, 1999.
[2] T. Ercit, Miner. Petrol. 43, **3**, 217-223, 1991.
[3] S. Pérez-Walton, *et al*, Phys. Status Solidi B 250, **8**, 1644-1650, 2013.