A first-principles study of P-Nb_2O_5

C. Valencia-Balvín[1*], S. Pérez-Walton [2], J. Peralta-Camposano[3] and J. M. Ososrio-Guillén[4]
[1]Facultad de Ingenierías, Institución Universitaria-ITM, Medellín, Colombia
[2]Universidad Andrés Bello, Santiago, Chile
[3]Instituto de Física, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia
*camilovalencia@itm.edu.co

Abstract

Niobium pentoxide is a wide gap semiconductor with a high dielectric constant and low dielectric loss, which make this compound very attractive for different electronic and optical applications. In this work, we present a study of the crystallographic and electronic properties of the P-Nb_2O_5 phase [1,2] from first-principles calculations within the framework of the Density Functional Theory using of the GGA-PBEsol parametrization [3], where the Kohn-Sham equations were solved using the projector augmented plane wave method implemented in the VASP code [4]. We have calculated the formation energy ($\Delta H = -20.84$ eV) and the Kohn-Sham indirect band gap (1.56 eV); where we have found that the valence band is located along the high symmetry direction $< u, u, \frac{1}{2} - u >$ and it is built up from the hybridization between O *p*-states and Nb *d*-states, while the conduction band is located at Γ and it is built up mainly by Nb *d*-states.

Table I. Experimental and calculated lattice parameters (Tetragonal structure, space group $I4_122$).

	a(Å)	c(Å)	V(Å^3)
Experimental	3.896	25.43	385.997
Calculated	3.7400	27.2522	381.19

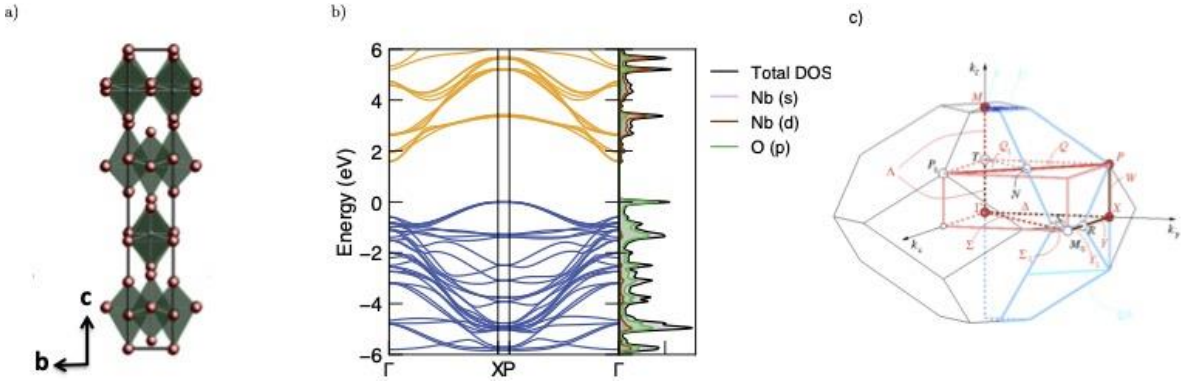

Figure 1: a) P-Nb_2O_5 unit cell, where the Nb atoms (green balls) are surrounded by 6 O atoms (red balls), forming a chain of distorted octahedra that share O atoms. b) Calculated electronic structure. C) First Brillouin Zone

References

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