Effect of polaron formation on electronic, charge and magnetic properties of $Nb_{12}O_{29}$

D. B. Migas [1],

A. B. Filonov [2],

V. E. Borisenko [3],

N.V. Skorodumova (Foreign) [4]

1, 3 Belarusian State University of Informatics and Radioelectronics, P. Brovka 6, 220013, Minsk, Belarus; National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe Shosse 31, 115409, Moscow, Russia

2 Belarusian State University of Informatics and Radioelectronics, P. Brovka 6, 220013, Minsk, Belarus

4 Foreign (Multiscale Materials Modelling, Department of Materials and Engineering, Royal Institute of Technology (KTH), SE-10044, Stockholm, Sweden; Department of Physics and Astronomy, Uppsala University, Box 516, SE-75121, Uppsala, Sweden)

Keywords: Substoichiometric niobium oxides, Polaron, Charge and magnetic ordering.

Abstract: We present the *ab initio* study of different phases of $Nb_{12}O_{29}$, which has been done in the framework of density functional theory

using the onsite Hubbard-U correction applied to the Nb-d states. We vary the U parameter in between 0 and 7 eV and suggest U = 3.7–5.0 eV to be most appropriate for the description of $Nb_{12}O_{29}$. We show that one cannot get any adequate description of this oxide using the crystallographic unit cell but at least 3 times larger supercell is needed increased along the shortest lattice parameter *b* to accommodate lattice distortions associated with polaron formation. Our results obtained for the enlarged cells show the possibility of simultaneous co-existence of localized states (polaron formation) and delocalized states providing metal-like properties of $Nb_{12}O_{29}$, in qualitative agreement with available experimental data.

This article published in: Effect of polaron formation on electronic, charge and magnetic properties of $Nb_{12}O_{29}$ / D. B. Migas [and others] // Journal of Alloys and Compounds – 2020. – Vol. 821, № 9. – P. 153527. https://doi.org/10.1016/j.jallcom.2019.153527.

Internet link to this article:

https://www.sciencedirect.com/science/article/abs/pii/S0925838819347735 .