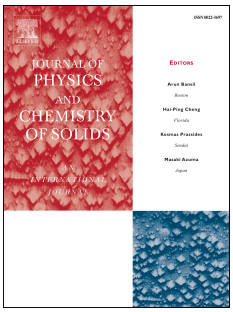
Accepted Manuscript



Optical properties of $B_{12}P_2$ crystals: Ab initio calculation and EELS

V.V. Reshetniak, B.N. Mavrin, V.V. Medvedev, I.A. Perezhogin, B.A. Kulnitskiy

PII: S0022-3697(17)31908-X

DOI: 10.1016/j.jpcs.2018.02.005

Reference: PCS 8419

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 9 October 2017

Revised Date: 22 January 2018

Accepted Date: 2 February 2018

Please cite this article as: V.V. Reshetniak, B.N. Mavrin, V.V. Medvedev, I.A. Perezhogin, B.A. Kulnitskiy, Optical properties of $B_{12}P_2$ crystals: Ab initio calculation and EELS, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.02.005.

Optical properties of $B_{12}P_2$ crystals: ab initio calculation and EELS

V.V. Reshetniak[1,2], B.N. Mavrin[2], V.V. Medvedev[2],
I.A. Perezhogin[3,4,5], B.A. Kulnitskiy[3,4]

[1]'RnD-ISAN' LLC, ul. Promyshlennaya 1A, 142191 Moscow, Troitsk, Russia; v.reshetnyak@rnd-isan.ru;

[2]Institute for Spectroscopy, Russian Academy of Sciences, ul. Fizicheskaya 5, 108840 Moscow, Troitsk, Russia;

[3]Technological Institute of Superhard and New Carbon Materials, ul. Tsentralnaya 7a, 142190 Moscow, Troitsk, Russia;

[4]Moscow Institute of Physics and Technology (State University), Institutskii per. 9, 141701 Dolgoprudnyi, Russia;

[5]M.V. Lomonosov Moscow State University, Leninskie Gory, 119991 Moscow, Russia

Abstract*. We report an experimental and theoretical investigation of the electronic structure and optical properties of $B_{12}P_2$ crystals in the energy range up to 60 eV. Experimental studies are performed by the method of electron energy loss spectroscopy, and theoretical studies are carried out using density functional theory and the GW approximation. The calculated dependence of the energy loss function is in agreement with the experiment. Based on the results of the calculations, we determine the optical properties of $B_{12}P_2$ crystals and investigate their anisotropy. The dispersion and density of electronic states are calculated and analyzed.*

Keywords: boron rich solids, boron subphosphide, EELS, DFT, TDDFT, ab initio, GW, electronic structure

1. Introduction

Icosahedral boron-rich crystals have recently attracted great interest of researchers due to their potential use in various applications. Rhombohedral α-B_{12} crystals have the simplest structure among these compounds. They belong to the space group symmetry D_{3d}^5 = R3m and consist of slightly distorted boron icosahedra located at the vertices of the unit cell. Each icosahedral cluster is made of six polar (three boron atoms in the upper part of the icosahedron and three atoms in the lower part) and six equatorial atoms. Neighboring icosahedra are linked by two-center bonds between polar atoms and three-center bonds Δ between equatorial atoms (Figs. 1a – 1c).

Crystals of boron subphosphide, boron subnitride, boron subarsenide, and boron subsulphide are characterized by a similar structure in which impurity atoms involved in the interaction between neighboring icosahedrons are embedded at the sites of the Δ bonds. Figures 1d – 1f show the stoichiometric structure of $B_{12}X_2$ crystals, where X is the doping atom. This stoichiometric structure is typical of boron suboxide, boron subphosphide, boron subsilicide, boron subarsenide, and boron subsulphide [1,2]. For boron subnitride, however, along with the foregoing, there are other model structures in which atomic chains between icosahedra consist of three atoms (N – B – N), or the structure contains both two- and three-atom chains [3–5]. Boron carbides also have a similar