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Electronic structure of alumina doped by light elements

M.A. Korotin* and E.Z. Kurmaev

M.N. Mikheev Institute of Metal Physics, Ural Division of Russian Academy of Sciences, 620108 Yekaterinburg, Russia

*Corresponding author, e-mail: michael.korotin@imp.uran.ru

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Abstract. The results of calculations of electronic structure and magnetic properties of α-Al_2O_3 doped by light elements (B, C and N) are presented. All calculations were performed within the density functional theory in the coherent potential approximation. Several possibilities of the 6 at. % impurities distribution were considered: nitrogen, carbon and boron impurities (marked as X in the general case) in oxygen sublattice – $Al_2[O_{0.98}X_{0.02}]_3$, in interstitials – $Al_2O_3X_{0.06}$, both in oxygen sites and interstitials – $Al_2[O_{0.99}X_{0.01}]_3X_{0.03}$. For each case, the calculations were performed for nonmagnetic as well as magnetic states of the impurity atoms. It is found that both for substitutional and interstitial impurities all sp-element impurities induce spin-polarized states around the Fermi level and reduce the band gap in Al_2O_3.

1. Introduction

The ceramic materials are widely used in mechanical and functional applications, and now be crucial materials to support the modern technologies. Alumina or aluminum oxide (Al_2O_3) in its various levels of purity is used more often than any other advanced ceramic materials [1]. It has been used for decades in electrical components for its high electrical insulation [2], and also in mechanical parts for its high strength, and corrosion- and wear-resistance [3-5]. The corundum phase of alumina (α-Al_2O_3), which has a broad bandgap (8.3 eV), is widely used in optical devices. In the past two decades, a large amount of research has been devoted to the optical properties of materials based on α-Al_2O_3. Many of these properties are closely related to point defects, especially oxygen vacancies and impurities introduced in bulk α-Al_2O_3. It was found to be very efficient (comparing with other dopants, such as Ti, Mg, Y, Cr and Ni (see references in [6])) to introduce carbon impurities to aluminum oxide for enhancement of luminescent sensitivity for radiation dosimetry [7]. Now the C:Al_2O_3 is widely used in thermoluminescence dosimetry (TLD) and optically stimulated luminescence dosimetry (OSLD) [8-9]. In comparison with other luminous materials (such as doped LiF, GaF_2, and $GaSO_4$), carbon doped Al_2O_3 has the advantages of high sensitivity, wide linear dose response range (10^{-7} to 10 Gy), and low