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THE ROLE OF INTRINSIC DEFECTS IN OPTICAL PROPERTIES OF β-Ga_2O_3 CRYSTAL. AB INITIO STUDIES.

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Gallium oxide (β-Ga_2O_3) is emerging as a viable candidate for certain classes of power electronics, solar blind UV photodetectors, solar cells, and sensors with capabilities beyond existing technologies due to its large bandgap [1-5].

Currently, the lack of understanding and control of the unintentional *n*-type conductivity of β-Ga_2O_3 still inhibits its applications. As with many other oxides, this conductivity has historically been attributed to the presence of oxygen vacancies V_O, largely based on the correlation between conductivity and oxygen partial pressure in annealing environments. Calculations have offered insight into the migration mechanisms and the relative energies of oxygen vacancies in the inequivalent sites of the monoclinic structure but only minimal information about the charge states and ionization energies.

So, we report results of the *ab initio* LCAO calculations of optical charge transition levels of native and impurity defects in Ga_2O_3 crystal. As impurity the atomic hydrogen in interstitial and oxygen vacancy positions (H_i and H_O) has been considered. We used hybrid DFT method (B3PW exchange-correlation functional) as incorporated into the CRYSTAL computer code [6] using the supercell model and linear combination of atomic orbitals (LCAO) basis set. These computational set provide good approximation of basic properties of pure Ga_2O_3, in particular mach better prediction of direct bandgap than standard GGA functionals (4.58 eV vs 2.3 eV) that comparable with experimental value of 4.9 eV [7].

Formation energies E_f are key quantities from which we can derive impurity and defect concentrations, stability of different charge states, and the related electronic transition levels. Errors due to spurious electrostatic interactions in the finite-sized cells were corrected using the scheme proposed by Leslie and Gillan [8] and by Makov and Payne [9].

As results we suggest that V_O acts as a deep donor with transition levels more than 1 eV and cannot contribute to n-type conductivity. Moreover, formation energy of V_O is high enough excludes high concentration of these defects in crystal. On the other hand, we find that hydrogen impurity can be easily incorporate to crystal due its low formation energy and migration barrier. The calculated transition states of hydrogen both in vacancy and interstitial positions indicate its shallow donor character. Thus, the presence of hydrogen in Ga_2O_3 crystal good explains persistence n-type conductivity. Our calculated results are fully consistent with other computational studies [10 and references therein].

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