TRANSITION LEVELS OF ACCEPTOR IMPURITIES IN ZNO CRYSTAL BY DFT-LCAO CALCULATIONS

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It is known that zinc oxide is a promising functional material for optoelectronics, in particular for LEDs. Today, there are many experimental and theoretical studies devoted to the study of the electronic structure of zinc oxide doped with donor and acceptor impurities [1, 2]. In particular, it became clear that the group V impurities do not play an important role in the production of the p-type semiconductor. However, here, the mechanism of conductivity of a doped crystal remains unclear, since it does not have a detailed description. The answer to the question about mechanism of influence of various impurities on conductivity has no direct experimental proofs, but is formulated from direct observations. In this connection, there arises the need for a detailed description of the electronic properties of the equilibrium crystal structure with an impurity of a certain type.

We present the results of DFT-LCAO calculations of the optical transition levels for nitrogen and phosphorus elements, introduced to zinc oxide crystal. The calculations are carried out in the CRYSTAL program [3]. Errors due to spurious electrostatic interactions in the finite-sized cells were corrected using the scheme proposed by Leslie and Gillan [4] and by Makov and Payne [5].

As result we shown that nitrogen and phosphorus are rather deep acceptors than small ones with optical transition levels ε(0/-) about ~2.0 and 2.2 eV for N and P, respectively, and do not contribute to p-type conductivity of ZnO. As shown by a recent combined EPR and DFT/B3LYP study, nitrogen species indeed are rather deep acceptors, confirming the results of our calculations [6]. It has been shown that N_O with the hole localized along the bond parallel to the c axis ($N_{O\|}$) is the most stable configuration and gives good agreement with electron paramagnetic resonance (EPR) measurements [6].This should be enough to disregard the X_O (X=N, P) configurations as a possible source of p-type doping.

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