The study of formation energy for ZnO native defects and their interaction with donor Al impurity in ZnO by the help of fullerene like model

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For the development technology of growing for the control of properties for ZnO based materials doped by Al and other donor impurities for their applications in photovoltaics and optoelectronic devices, the minimization of donor impurities compensation by native acceptor defects (V_{Zn}, O_i etc.) is required. We successfully used fullerene like (FL) cluster model earlier for a solution of the band engineering problems in ZnO alloys and precipitation of CdO phase in these materials[1-3].

The aim of this work is a determination of influence the native defect Oi as well as stacking fault defects in ZnO lattice on electroactivity of AL impurity by applying fullerene-like model with FL $Zn_{36}O_{36}$ cluster. This cluster was chosen as a model at ab initio quantum-chemical investigations due to report about obtaining ZnO isolated clusters at laser ablation of zinc peroxide. Our recent development for investigation of FL $Zn_{32}Al_4O_{36}$ clusters is presented in [4]. The geometry and electron density distribution is shown on Fig.1.

The calculations of optimized geometry, full energy and electronic structure were fulfilled in the frames of electronic density functional theory with B3LYP hybrid functional with the MINI basis set. The calculations showed that Al impurity has a tendency to be situated in the vicinity of stacking faults of ZnO lattice. In this case the electroactivity of Al impurity increases. Oi displacement near a stacking fault in ZnO lattice and Al impurity results in essential lowering of the Oi formation energy. Thus this defect becomes the leading one. Its ionization energy increases in comparrizon with the situation when Oi is situated near Al atom, but far from the stacking fault.

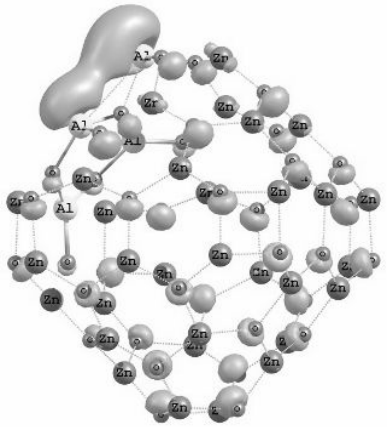

Fig.1. The geometry of the $Zn_{32}Al_4O_{36}$ cluster; Electronic density of upper filled molecular orbit (HOMO) is situated near Al impurity.

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[3] I.I. Shtepliuk, V. Khranovskyy , G. Lashkarev, et al., *Solid-State Electronics,* **81**, 72-77 (2013)
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