Study of donor Al impurity by the help of fullerene like model

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Fullerene like model (FLM) was used successfully by us earlier for a solution of band engineering problems in $Zn_{1-x}Cd_xO$ alloys and precipitation of CdO phase in this matrix [1-4].

For technology of growing and control of properties for film materials based on ZnO doped by Al and their applications in photovoltaic and optoelectronic devices the minimization of self-compensation of donor impurity by intrinsic acceptor defects (V_{Zn}, O_i etc.) is required. Exponential dependence of defect concentration on their formation energy shows, that in any crystal the only almost defects with minimal energy are present. For determination of dominating defects we started the series of computational experiments.

The basic model of isolated FL $Zn_{32}Al_4O_{36}$ cluster was formed. In this cluster four three-valent Al atoms substitute two-valent Zn in its cation sublattice. This cluster has zero charge. Its electronic structure was investigated. The computation of optimized geometry, full energy and the value of forbidden zone was fulfilled in the frames of functional B3LYP electronic density method with basis set 6-31G(d). Energy gap between Al level and the conduction band was evaluated as 80 meV. This ionization energy agrees satisfactorily with experimental value calculated from the temperature dependence of Hall coefficient (60 meV) [5].

Thus FLM provided again its capable of living, what allows to use it in future for investigation the electroactivity of donor impurities of the third group due to their compensation by intrinsic acceptor defects of ZnO crystal lattice.

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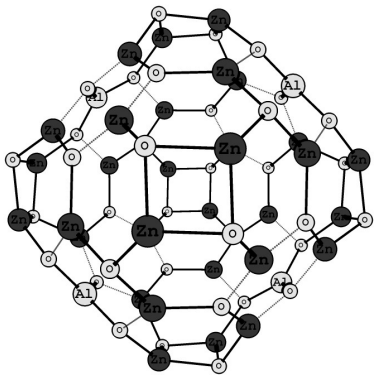

Fig.1. Optimized geometry of the $Zn_{32}Al_4O_{36}$ cluster.

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