“Nanocomposites and nanomaterials”

First principle study of native point defects in ZnO nanoclusters

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We present the results of *ab initio* density functional theory studies of native point defects properties of “magic” clusters $(ZnO)_n$ (n = 34, 60). Calculations were performed using ultrasoft pseudopotentials in the basis of plane waves, similar to previous studies [1]. The exchange-correlation functional is a generalized gradient approximation (GGA) proposed by Perdew, Burke and Ernzerhof. Optimization of the nanocluster structure was performed using conjugate gradient method. No symmetry restrictions were used during structure optimization.

We performed geometry optimization and energy calculations for a number of isomers of $(ZnO)_{34}$ and $(ZnO)_{60}$ nanoclusters with O and Zn vacancies, as well as, interstitials and antisites, and compared the results with the values obtained in our previous studies for ZnO nanoclusters without defects [2].

Analysis of the obtained results showed that in case of zinc-rich conditions the oxygen vacancies are predominant defects; under oxygen-rich conditions the oxygen interstitials and zinc vacancies are the main defect types. The analysis of the electronic properties of these clusters show a significant reduction of the width of the band gap which could be explained by the emergence of transition levels formed mainly by the intrinsic defects. Transition levels near the bottom of the conduction band consist mainly from zinc interstitials and oxygen vacancies, while zinc vacancies and oxygen interstitials occupy mostly valence band maximum.

1. *Bovgyra O.V., Bovhyra R.V., Kovalenko M.V., Popovych D.I., Serednytski A.S.* Density functional theory study of structural and electronical properties of ZnO clusters // Journal of Nano- and Electronic Physics.-2015.-**7,** N 4.-P. 04090-1–04090-6.

2. *Bovgyra O.V., Bovhyra R.V., Popovych D.I., Serednytski A.S.* Ab inito study of structural and electronic properties of $(ZnO)_n$ “magical” nanoclusters n=(34, 60 // Nanoscale Research Letters.-2017.-**12:76.**