“Nanocomposites and nanomaterials”

Ab initio study of structural and elecronical properties of ZnO nanoclusters

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We present results of *ab initio* density functional theory studies of energy spectrum and ground stage parameters 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.

In order to determine the most stable structure for the "magic" clusters $(ZnO)_{34}$ and $(ZnO)_{60}$ we examined a number of isomers. Among them were fullerene-like hollow structures that satisfy the rule of six isolated quadrangles. Also, frame layered structures $(ZnO)_6@(ZnO)_{28}$ and $(ZnO)_{12}@(ZnO)_{48}$ were built. Finally zeolite-like structures built from $(ZnO)_{12}$ structural units were examined.

To analyze the stability of ZnO clusters we calculated binding energy per one molecule of ZnO. Analysis of the energy values shows that in case of $(ZnO)_{34}$ nanocluster the most energetically favorable is fullerene-like hollow structure. All such structures, that satisfy the rule of isolated quadrangles, have approximately the same binding energy. Among the structures in the form embedded clusters more stable are those in which the interatomic distance between the outer and inner shell is greater, i.e. intra cluster interactions are stronger than interaction force between the clusters. In the case of $(ZnO)_{60}$ nanoclusters the most stable is the zeolite-like type of structure which consists of eight nanoclusters $(ZnO)_{12}$ that have joint quadrangle edges.

1. *Bovgyra O.V., Bovhyra R.V., Kovalenko M.V., Popovych D.I., Serednytski A.S.* Density functional theorystudy of structural and electronical propertiesof ZnO clusters // Journal of Nano- and Electronic Physics.-2013.-**5,** N 1.-P. 1027