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 $(ZnO)_n$ ($n = 34$). 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.

The ab initio study of ZnO crystals is quite difficult. First, the structure of wurtzite contains twice as many atoms in the unit cell than zincblende structure. Second, oxygen and zinc are so-called "problem" atoms in terms of building their pseudopotentials. In both cases, the valence orbitals of O 2p and Zn 3d don't have core partners with the same orbital angular momentum and as a result are strongly bound, which require a larger basis of plane waves to describe them.

In order to determine the most stable structure for the "magic" clusters $(ZnO)_{34}$ 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 $(ZnO)_6@(ZnO)_{28}$ were built.

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.

4. О.В. Бовгира. Вивчення структурних та електронних властивостей кластерів ZnO методом теорії функціонала густини. // *Журнал нано- та електронної фізики.* – 2013. – Т.**5,** №1. – С. 01027-1–01027-6.