Magic Clusters of ZnO

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Stable / magic clusters sized between molecules and solid state attract much attention both from fundamental science, as specific objects of unique structure and unusual properties, and from applied science, as perfect probes and promising building blocks for assembling of nanostructures. Among the variety of materials, clusters of zinc oxide are of particular interest due to their size-dependent optical properties and implied novel applications in solar energy conversion, optoelectronics, and photochemistry. Moreover, ZnO is low toxic material that opens way for its application in medicine and biology.

ZnO is well known and deeply studied semiconductor material. However, its stable small clusters have been synthesized with atomic precision just recently (Dmytruk et al. Microelectron. J 40 (2009) 218), and now they are a subject of extensive investigations. Namely, essentially different from other II-VI group compounds features on its time-of-flight mass spectra obtained by pulsed laser ablation, stimulated us to perform computer simulations of their structure by quantum chemistry calculation methods. As a model, several cage-like structures have been considered (namely, known structures of carbon "onions", CdSe and BN, as well as other "handmade" structures constructed by simple chemical intuition), as well as fragments of the bulk wurtzite structure. Semiempirical (AM1, PM3) and first-principles (B3LYP functional for DFT on 6-31G and 3-21G basis sets) calculations confirm the enhanced stability of the clusters of onion-like structure over the bulk fragments.

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