Rings, Towers and Cages in Zn$_n$O$_n$ Clusters

ARTHUR REBER, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, Richmond Va. 23284, JAGTAR HUNJAN, MARCELA BELTRAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico — It is shown that the transition from an elementary ZnO molecule to compact bulk wurtzite ZnO proceeds via hollow rings, towers, and cages. First principles electronic structure calculations within a gradient corrected density functional framework have been carried out to investigate the progression of geometries and electronic properties of Zn$_n$O$_n$ \((n=2, 3, 4, 5, 6, 7)\) clusters. It is shown that Zn$_3$O$_3$ is particularly stable. Starting at Zn$_8$O$_8$, these elementary rings begin to assemble into column structures that begin to distort at \(n=10\). The ground states of Zn$_{12}$O$_{12}$, and Zn$_{16}$O$_{16}$ are single cages while the structure of Zn$_{11}$O$_{11}$, Zn$_{15}$O$_{15}$ and Zn$_{21}$O$_{21}$ can be described as barrels. The Zn$_{12}$O$_{12}$ cage has a high dissociation energy and a large highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) gap of 2.51 eV making it a potential candidate for cluster assemblies.

Shiv Khanna

Date submitted: 28 Nov 2005 Electronic form version 1.4