Rings, Towers and Cages in ZnₙOₙ 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 ZnₙOₙ (n=2,12,15,16,21) clusters. It is shown that ZnₙOₙ (n=2, 3, 4, 5, 6, 7) clusters are all single, highly stable rings and that Zn₃O₃ is particularly stable. Starting at Zn₈O₈, these elementary rings begin to assemble into column structures that begin to distort at n=10. The ground states of Zn₁₂O₁₂, and Zn₁₆O₁₆ are single cages while the structure of Zn₁₁O₁₁, Zn₁₅O₁₅ and Zn₂₁O₂₁ can be described as barrels. The Zn₁₂O₁₂ 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.