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Rings, Towers and Cages in Zn_nO_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_nO_n (n=2-12,15,16,21) clusters. It is shown that Zn_nO_n (n=2, 3, 4, 5, 6, 7) clusters are all single, highly stable rings and that Zn_3O_3 is particularly stable. Starting at Zn_8O_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

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