Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Fullerene Molecules and Other Clusters of III-V Compounds AJIT HIRA, JOHN AUXIER II, MELINDA LUCERO, Northern New Mexico College — The goal of the our work is to derive geometries of fullerene-like cages and other clusters of atoms from groups III and V of the periodic table. Our previous research focused on Carbon Fullerenes and on Ga_nAs_n clusters (n = 1 thru 12). Our research group has made an original discovery about Ga_nAs_n clusters. In our work on nanotechnology to date, we used the hybrid ab initio methods of quantum chemistry to derive the different geometries for the clusters of interest. We also calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps, and IR spectra for these geometries. Of particular significance was the magic number for GaAs cluster stability that we found at n = 8. This is important because materials containing controlled III-V nanostructures provide the capability of preparing new classes of materials with enhanced optical, magnetic, chemical sensor and photo-catalytic properties. The second phase of the investigation will examine the effects of confinement on the optical properties the clusters. It will be interesting to observe novel linear as well as nonlinear optical processes in them. The third phase of the investigation will focus on the improved design of solar cells based on the optical properties of the clusters.

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Date submitted: 20 Nov 2009 Electronic form version 1.4