Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Theoretical Spectra and Optimization of Geometries of GaAs Clusters AJIT HIRA, JOHN AUXIER, Northern New Mexico College, MATILDA FERNANDEZ, New Mexico Highlands University — The goal of the current research is to expand our previous work on Ga_nAs_n clusters (n = 1 thru 12) and on gallium arsenide nanostructures. Our research group appears to be on the verge of making an original discovery about these clusters, which we want to disseminate through publication in a professional journal. So far in our work on nanotechnology, we used the hybrid ab initio methods of quantum chemistry to derive the optimal geometries of the Ga_nAs_n clusters for n going from 1 to 12. We also calculated binding energies, bondlengths, ionization potentials, electron affinities and HOMO-LUMO gaps, and IR spectra for these geometries. Of particular significance is the magic numbers for GaAs cluster stability that we found at n =8, 10, 12 and 16. Also, we recovered 32.7 % of the bulk cohesive energy of 6.67 eV at 2.18 eV for n =10. However, we need to validate the accuracy of our results through more sophisticated computation and through experimental work. This is important; because materials containing controlled GaAs nanostructures provide the capability of preparing new classes of materials with enhanced optical, magnetic, chemical sensor and photocatalytic properties. The second phase of the investigation will examine the effects of confinement on the optical properties the Ga_nAs_n clusters.

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Date submitted: 15 Dec 2008 Electronic form version 1.4