Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Theoretical Study of Chemisorption on GaAs Clusters.[1] ALEXANDRA VALDEZ, AJIT HIRA, RUBEN RIVERA, AMBERLY MAES, Northern New Mexico College — We extend our work on the theoretical study of molecular clusters in this report on the chemical properties of small Ga_nAs_n clusters (n = 2 - 14). We study the chemisorption of different atomic and molecular species on small clusters of semiconducting elements, by examining the interactions of O_2, O_2, Li, and Be adsorbates with the GaAs clusters. Semiconductor clusters are of interest for the understanding of quantum size effects and of metallization phenomena. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) were used to derive optimal geometries for the clusters of interest. We compared calculated binding energies, bond-lengths, ionization potentials, electron affinities, and HOMO-LUMO gaps for these clusters. Mapping of the singlet, triplet, and quintet, potential energy surfaces was performed. Implications for fundamental mechanisms of atomistic assembly on the GaAs surfaces will be examined. Applications to the manufacture of GaAs nanowires will be presented.

[1]Research supported by the NSF-funded New Mexico AMP program

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Date submitted: 06 Jan 2017 Electronic form version 1.4