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Interactions of Ga_nAs_n Clusters with CGaAs Cages: Possible Nanostructures A.S. HIRA, E. ALLISON, M.F. FERNANDEZ, J. SHIPMAN, E.R. VELARDE, Northern New Mexico College — Extending our work on fullerene-alkali complexes[1], we now examine the interactions of small Ga_nAs_n clusters (n = 1 thru 10) with mixed CGaAs cage clusters. First, we derive the physical and chemical properties of the GaAs clusters, including their binding energies, bondlengths, ionization potentials and charge distributions. The geometries of the small gallium arsenide clusters are based on full optimizations. Electron correlation effects are included for binding energies and optimal intermolecular bondlengths. Next we focus on the physical and chemical properties of 60-atom mixed CGaAs cages. The optimization of the cages is subject to symmetry constraints. The third phase of the investigation examines the interactions of the small GaAs clusters with the CGaAs cages. For these complexes various properties, including dissociation channels and dissociation energies, are tabulated. We also explore the implications of this research for the design of nanostructures. 1. Daniel Bulnes, Nichole Moya-Leyba, Erica Velarde and Ajit Hira, " Theoretical Study of Na_3C_{60} and Na_4C_{60}Clusters: Pathways to Nanoscale Contacts", *Bull. Am. Phys. Soc.* 50, 1475 (March 2005).

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