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Quantum Mechanics of Chemisorption on GaAs Clusters[1] FRANK NARANJO, AJIT HIRA, RUBEN RIVERA, OLIVER OVIEDO, Nothern New Mexico College — This research focuses on the theoretical study of molecular clusters to examine the chemical properties of small Ga_nAs_n clusters (n = 2 - 10). We study the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of H, H_2, Li and Be adsorbates with the GaAs clusters. Semiconductor clusters are of interest for the study of quantum size effects and for metallization phenomena, Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare 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 is performed. Implications for fundamental mechanisms of atomistic assembly on the GaAs surfaces are examined.

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