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PREDICTED STRUCTURES AND ELECTRONIC PROPERTIES OF GALLIUM-INDIUM CLUSTERS Ga_mIn_{n-m} (n = 4, 6, 8 AND $m < n$): A DENSITY FUNCTIONAL STUDY*

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Various structural possibilities for small gallium-indium Ga_mIn_{n-m} (n = 4, 6, 8 and $m < n$) clusters are investigated using the density functional theory (DFT) method at the B3LYP/TZP level. The optimized structures tend to prefer compact structures, wherein the trigonal prism and rhombic prism configurations are favoured for n = 6 and 8, respectively. The bonding energy per atom is calculated according to the cluster size. The HOMO-LUMO gaps, ionization potentials, electron affinities, and chemical hardness (η) are also computed for the most stable isomers of each cluster and used to predict their relative stabilities. The obtained results indicate that the Ga-rich clusters are more stable than the In-rich ones with the same total number of atoms. The Ga–Ga bond is stronger than the Ga–In bond and the latter is stronger than the In–In one. Therefore, the Ga_7In cluster is relatively the most stable structure. The relative reactivity of Ga_mIn_{n-m} (n = 4, 6, 8 and $m < n$) clusters could be predicted based on the chemical hardness. The computed large HOMO-LUMO gap energies could be used as an index of the kinetic stability for the studied clusters.

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