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Structural and electronic properties of Gen and EuGen-1 nanoclusters: A full potential DFT study

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Abstract

In this work, the stability, structure and electronic properties of the nanoclusters of germanium (Ge_n) and europium atom doped germanium clusters ($EuGe_{n-1}$) with n=2 to 12, 15 and 20 were investigated. First, the stability of nanoclusters such as Ge_n and $EuGe_{n-1}$ was addressed using FHI-aims as a software package based on the density functional theory. Then the lowest-energy structures were selected for calculating the first vertical ionization with the symmetry adapted cluster-configuration interaction General-R (SAC-CI-General-R) method. The results of this research show that there is a good agreement between calculation and experiment ionization potential for Ge_n nanoclusters. Generally, the analyses of binding energies show that increasing the size of nanoclusters leads to more stability for nanoclusters. The most stable nanoclusters for $EuGe_n$ can be created with exchanging the Eu atom in the most stable Ge_{n+1} nanoclusters, but there is an exception for n=11 case. Here, the second difference in energy (Δ_2E) and gap energy are computed for the stable nanoclusters. The results of ionization energy and second difference in energy confirm that Ge_7 and Ge_{10} also $EuGe_8$ and $EuGe_{10}$ have the most stability.

Keywords: germanium nanoclusters, fhi-aims, full potential, first ionization energy, second difference in energy, gap energy

For full article, refer to the Persian section