Structures and Electronic Properties of $B_3Si_n^-$ (n=4-10) Clusters:

A Combined Ab Initio and Experimental Study

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Boron-doped silicon cluster anions, $B_3Si_n^-$ (n=4-10), have been generated by laser vaporization and investigated by anion photoelectron spectroscopy. The vertical detachment energies (VDEs) and adiabatic detachment energies (ADEs) of these clusters were obtained. Meanwhile, genetic algorithm combined with *ab-initio* density functional theory (GA-DFT) calculations are employed to determine their ground state structures systematically. GA-DFT is a method that developed autonomously by Zhao et al.. And yet Genetic algorithm (GA) is an effective way to search the ground-states of clusters. Excellent agreement is found between theory and experiment. Among the $B_3Si_n^-$ clusters, $B_3Si_9^-$ is relatively more stable. Generally speaking, three B atoms tend to form triangle surrounded by Si atoms and form strong B−B bonds.

Keywords: doped silicon clusters, low-energy structures, genetic algorithm.

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