

Modified genetic algorithms to model cluster structures in medium-sized silicon clusters: Si₁₈ - Si₆₀

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This paper presents the results obtained using a genetic algorithm (GA) to search for stable structures of medium-size silicon clusters. This is the third report in which a GA coupled with the MSINDO semiempirical molecular orbital program is used to find stable atomic cluster structures. The structures selected by the GA-MSINDO method were further optimized using the density functional theory (DFT). This combination of GA-MSINDO global optimization followed by DFT local optimization proves to be very effective for searching the structures of medium-size Si clusters. For most of the clusters studied here we report different structures with significant lower energy than those previously found using limited search approaches on common structural motifs. This demonstrates the need for global optimization schemes when searching for stable structures of medium-size silicon clusters. © 2006 The American Physical Society.