Modified genetic algorithms to model cluster structures in medium-size silicon

clusters

Bazterra, Victor E.

Oña, Ofelia

Caputo, María C.

Ferraro, Marta B.

Fuentealba, Patricio

Facelli, Julio C.

Genetic algorithms (GA) were used to investigate the stable isomers of silicon clusters. In order to find the cluster structures, a semiempirical energy function was used by the GA that were further optimized using density-functional theory. A different structure with a significantly lower energy was found in the case of Si36. The need for global optimization schemes rather than local optimization was demonstrated by the results while searching for stable structures of medium-size silicon clusters.