A Fukui function-guided genetic algorithm. Assessment on structural prediction of Sin (n = 12?20) clusters

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Theoretical studies are essential for the structural characterization of clusters, when it comes to rationalize their unique size-dependent properties and composition. However, the rapid growth of local minima on the potential energy surface (PES), with respect to cluster size, makes the candidate identification a challenging undertaking. In this article, we introduce a hybrid strategy to explore the PES of clusters. This proposal involves the use of a biased initial population of a genetic algorithm procedure. Each individual in this population is built by assembling small fragments, according to the best matching of the Fukui function. The performance of a genetic algorithm procedure. The performance of the method is assessed on the PES exploration of medium-sized Sin clusters (n = 12?20). The most relevant results are: (a) the method converges at almost half of the time used by the canonical version of the GA and, (b) in all the studied cases, with the exception of Si13 and Si16, the method allowed to identify the global minimum (GM) and other important low-lying structures. Additionally, the apparent deficiency of the proposal to identify the GM was corrected when a Si atom, or other low-lying isomers, were considered to build the clusters. © 2017 Wiley Periodicals, Inc.

clusters

Fukui function

genetic algorithm

potential energy surface exploration

Genetic algorithms

Isomers

Molecular physics

Potential energy

Potential energy surfaces

Quantum chemistry

Silicon

Biased initial population

Candidate identifications

Clusters

Fukui functions

Guided genetic algorithms

Low-lying structures

Structural characterization

Theoretical study

Clustering algorithms

article

clinical article

genetic algorithm

human

human experiment

isomer

prediction

theoretical study