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New genetic algorithm paradigms applied to atomic and molecular clusters studies

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Abstract: New global optimization tools for atomic and molecular clusters studies are constantly been produced [1-4]. It is known that clusters have unique properties, which are difficult to predict using only chemical intuition, so, computational tools can help these studies. Among the current global optimization techniques, genetic algorithms stands out in obtaining the most stable geometry of atomic and molecular clusters. In this work, a study of six specific genetic operators was performed to obtain the most stable geometry of clusters. From these operators, the spherical crossover [4] and cut-and-splice crossover [5] are specific for genetic algorithms. The other four: angular operator, surface angular operator, geometric displacement and twist operator were initially proposed for Basin Hoping technique [1], and, in this work, were implemented in our group's genetic algorithm [2]. In addition, we propose a new paradigm that allows to manage these operators. This paradigm consists in increasing or decreasing the rate of creation of new individuals on the fly. Operators that are generating unstable structures have their creation rate reduced in the next genetic algorithm generation. Likewise, operators who are building structures that approach the global minimum have their creation rate increased. With these operators, nine genetic algorithm arrangements were built, one arrangement for each of the operators alone, and three with management operators' paradigm. As a test of the methods, fifty global optimizations of a Lennard-Jones set containing twenty-six atoms were made for each of the methods. The performance measure was the mean number of optimizations that were required to reach global minimum. Results pointed out twist operator as the best operator. Also, that management operators' paradigm could improve the overall performance of the method.

Key-words: **Global optimization, atomic and molecular clusters, genetic algorithm.**
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