Optimizing a Genetic Algorithm

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In order to adequately model the properties of atomic clusters, it is of crucial importance, first find the most stable structure for a given composition. This issue is not trivial, due to the great number of possible geometries, specially when the number of atoms and the elements involved increases. One method that has been used to solve this problem is the so-called Genetic Algorithm [1]. The idea is that starting from an initial population, new structures are generated which are compared with the old ones and can displace them if they have lower energies. This allows to carry out the search for global minima selectively and systematically.

The group of R. Johnston has developed a Parallel Genetic Algorithm [2] which can generate and relax several new structures independently at the same time. Moreover, it can do the search in presence of a surface, allowing to find the most stable structure of the deposited cluster. Taking this as starting point we implement new ideas to expand its functionalities and make it more efficient.

The method is, in general, very robust and works acceptably well with a wide range of parameters. However, we have found several ways to optimize the search reducing the number of needed calculations and even the time of each relaxation, therefore diminishing the overall computational effort.

[1] R. L. Johnston, *Dalton Trans.* 4193-4207 (2003).
[2] A. Shayeghi, *et al., Phys. Chem. Chem. Phys.* **17**, 2104-2112 (2015).