An efficient and reliable method for global geometry optimization of atomic and molecular clusters

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Using several concepts from Evolutionary Computing and some new strategies, we have arrived at an algorithm that is able to locate global minimum structures of atomic and molecular clusters on empirical potential energy surfaces with high efficiency and reliability. Performance examples are shown for the model system of Lennard-Jones clusters up to 250 atoms, establishing a cubic scaling of the algorithm with cluster size. Finally, it is demonstrated how this method can be joined with state-of-the-art correlated ab-initio calculations, for the example of pure and mixed water clusters.