NWPEsSe: A General Algorithm for Global Optimization of Chemical Structures

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The problem of global optimization constitutes an important area of modern computational sciences. From the perspective of computational chemistry, the first steps in theoretical studies of chemical systems often rely on finding the most stable structure, i.e., the global minimum (GM) on its potential energy surface (PES). Researchers have been investing large effort to develop efficient global optimization algorithms for chemical structures.[1-4] However, many of these methods are limited by the number or types of atoms of the system, or the codes are not publicly available.

We have developed the artificial bee colony algorithm (ABC) for efficient global optimization of large and extended chemical structures.[5-7] It is inspired by the foraging behavior of bee colonies which have a strategy to look for the best nectar as their food source. The ABC algorithm has been tested for several systems of different chemical nature: unsupported or supported clusters, large cluster assemblies, and periodic structures. For instances, pure gold clusters Au , ligated clusters Au (P(CH)) , graphene oxide-supported and oxygen-defected rutile(110) surface-supported Au , and cluster assembles containing more than 1000 atoms [Co Te (PEt)][C] / were tested. In all cases, the ABC algorithm exhibited excellent performance. For extended/periodic systems, the optimized structures were compared to structures obtained with simulated annealing technics and in all cases the structures were very similar.

The algorithm has been included in ABCluster[5,6] and NWPEsSe[7] which are freely available and have interfaces to many quantum mechanical and molecular dynamics codes. The ABCluster has been used very successfully in many studies such as methane activation mechanism,[8] atmospheric chemistry,[9,10] lanthanide chemistry,[11] energy storage,[12] reaction mechanism exploration,[13] and design of biological[14] and metalorganic framework materials,[15] to mention a few. NWPEsSe also includes a force matching algorithm that allows us to move from DFT-based to classical molecular dynamics approaches for extended systems. ABCluster and NWPEsSe have interfaces to NWChem, CP2K, Gaussian, xTB, MOPAC, ORCA, Lammps, Gromacs, and DMol3.

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