Diversity driven unbiased search of minimum energy cluster configurations

J. Rogan, M. Ramírez, V. Muñoz, J. A. Valdivia, G. García, R. Ramírez and M. Kiwi

Abstract

The determination of the spatial distributions that atoms adopt to form condensed matter is a problem of crucial importance, since most physical properties depend on the atomic arrangement. This is especially relevant for clusters, where periodicity is nonexistent. Several optimization procedures have been implemented to tackle this problem, with ever increasing success. Here we put forward a search scheme which preserves as large a diversity as allowed by the use of phenomenological potentials, generating in an unbiased fashion a bank of configurations to be explored; a procedure we denominate diversity driven unbiased search (DDUS). It consists in the generation, using phenomenological potentials, of a data bank of putative minima rather than a single, or just a few, configurations which are based on the conformational space annealing method (CSA). All of the configurations in the bank are thereafter refined by means of DFT computations. Certainly, in spite of our efforts to generate a bank as diverse as possible, not all relevant structures might be included in it, since quantum effects are ignored. The procedure is applied to several examples of rhodium, palladium, silver, platinum and gold clusters, between 5 and 23 atoms in size. The main conclusion we reach is that unbiased search, among a significant number of candidates, quite often leads to rather unexpectedly low symmetry configurations, which turn out to be the lowest energy ones within our scheme.