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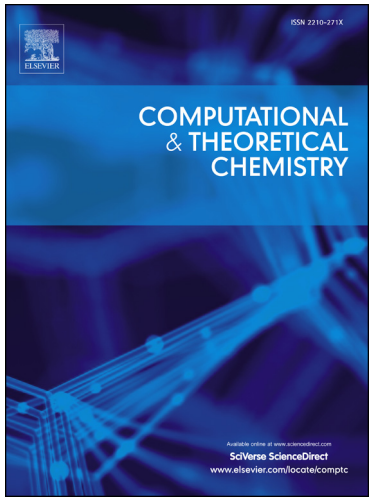

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Hybrid genetic-particle swarm algorithm: an efficient method for fast optimization of atomic clusters

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Abstract

In this paper, a new hybrid genetic-particle swarm algorithm with enhanced local search ability (L-GPS) has been proposed for the structural optimization problem. This algorithm combines the wide area search ability of the genetic algorithm, the local development capacity of the particle swarm optimization algorithm, the extremely strong local search ability of the limited memory quasi-Newton algorithm as well as the optimal switching point evaluation strategy for the self-adjustment of the global and local search. L-GPS achieves a faster convergence rate than the well-known stochastic methods for a large class of standard test functions. In addition, all the global minima of Lennard-Jones (LJ) clusters of 2 to 19 atoms are successfully and efficiently located. Moreover, the convergence rate is much faster than the well-known structural optimization methods. Our results indicate that L-GPS is a promising structural optimization algorithm for atomic LJ clusters.

Keywords: Structural optimization, Hybrid algorithm, Lennard-Jones cluster

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