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Cluster-based niching differential evolution algorithm for optimizing the stable structures of metallic clusters

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ABSTRACT

In this article, a cluster-based niching differential evolution algorithm, which combines the cluster pool, the niche method, and the differential evolution algorithm, has been employed to optimize the stable structures of iron clusters. The cluster pool is responsible for generation of the niche sub populations, and the differential evolutionary algorithm is used for the evolution of the population. A variety of mutation strategies have been applied in the algorithm instance. Moreover, the crossover operator of plane cut cross and the adjustment strategy make the algorithm more suitable for structural optimization of clusters. Subsequently, the performance of the algorithm has been examined by the effect of cluster pool size on the convergence speed and structural diversity. The accuracy and effectiveness of our algorithm have been verified by analyses of energy and structural evolutions. Finally, structural evolution of iron clusters with 3–80 atoms has been predicted by this algorithm.

1. Introduction

Metallic clusters have attracted great attention due to their potential applications in many fields such as physics, chemistry, biology and so on [1–4]. Among metallic clusters, iron (Fe) clusters are of considerable interest due to their exceptional magnetic properties such as ferromagnetism, high coercive force, low Curie temperature, high magnetic susceptibility. To date, Fe clusters have been extensively used in the aspects of giant magnetoresistance, magnetic recording, magnetic refrigeration, and magnetic probes [5]. As cheap metallic catalysts, Fe clusters have been widely used in Fischer-Tropsch reaction for producing hydrocarbon by using CO and H_2 in coal and natural gas. They can also be used as a cathode catalyst for fuel cell [6]. However, both the magnetic and catalytic properties of Fe clusters are strongly dependent on their structures. Therefore, an investigation on the structural properties of Fe clusters is crucial for understanding their physical and chemical performances.

Theoretically, to predict the structure of clusters is a typical global optimization problem. The optimization goal is to get the lowest-energy structure of clusters [7]. Essentially, exploring the stable structures of Fe clusters is to search the lowest energy of potential energy function. Usually, the potential energy function describes a potential energy surface of multi-dimensional space. The potential energy surface is considerably complex, thus searching the lowest energy on the potential energy surface is rather time-consuming. Furthermore, there are plenty of local minimum corresponding to metastable structures of cluster on the potential energy surface, the number of local minimum grows exponentially with the cluster size [8]. So far, many global optimization methods, such as heuristic algorithms and evolutionary algorithms, have been developed to optimize the structure of clusters. According to the number of individuals in the searching process, the algorithms can be divided into three categories: single individual searching algorithms, single population searching algorithms, and multi populations searching algorithms. Single individual searching algorithms, such as Monte Carlo method [9], Basin Hopping algorithm [10,11], simulated annealing algorithm [12], belong to simple searching algorithms. The search efficiency of these algorithms is poor due to the lack of repeatable search. Single population searching algorithms, such as genetic algorithm [13,14], particle swarm optimization algorithm [15,16], and artificial immune algorithm [17,18], are superior in comparison with the single individual searching algorithms because there exists the information exchange between different individuals in single population searching algorithms. However, they are apt to be trapped into the local optimum, leading to the premature convergence. Multi populations searching algorithms, including common pool [19], topology structure [20], and niche method [21], are able to improve the search capability of global optimization remarkably because they may maintain population diversity effectively and avoid

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the premature phenomena in single population searching algorithms.

In this article, we have proposed, for the first time, a cluster-based niching differential evolution algorithm to optimize the structure of Fe clusters by the multi populations searching algorithms with cluster-based niching method. As a first step, the effect of cluster pool size on convergence speed of algorithm and structural diversity has been analyzed. Secondly, the accuracy and effectiveness of the proposed algorithm have been verified by comparison experiments. Finally, we have examined the stable structures of Fe clusters with 3–80 atoms by using the proposed algorithm, and predict the evolutional law of stable structures with increasing cluster size. This article is structured as follows. Section 2 describes the potentials of Fe and the cluster-based niching differential evolution algorithm. Section 3 presents the calculated results and discussion. The main conclusions are summarized in Section 4.

2. Methodology

2.1. Potential description

In theoretical study of clusters, it is considerably important to accurately describe the interatomic interaction. In this work, the Finnis-Sinclair (FS) potentials [22], which are based on the second-moment approximation of the tight-bonding formulation, have been employed to describe the interaction between atoms in Fe clusters. The FS potentials represent many-body interactions, and their parameters are optimized to describe the lattice parameter, cohesive energy, elastic constants, vacancy formation energy, stacking-fault energy, and pressure-volume dependency. They have been confirmed to reproduce very well the basic structural and dynamics properties of Fe [23]. The total energy for a system of N atoms is given as

$$E_{tot} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} V_{ij}(r_{ij}) - A\sum_{i=1}^{N}\sqrt{\rho_i}, \tag{1}$$

where r_{ij} represents the distance between atoms i and j; ρ_i is the electronic charge density at the site of atom i, it can be expressed by

$$\rho_i = \sum_{j=1, i\neq j}^{N} \phi_{ij}(r_{ij}), \tag{2}$$

in which $\phi_{ij}(r_{ij})$ is a cohesive term related to the sum of squares of overlap integrals for the valance electrons, represents the contribution of electronic charge density for j atom to i atom, can be defined as

$$\Phi(r) = \begin{cases} (r-d)^2 & r \leqslant d \\ 0 & r > d \end{cases}, \tag{3}$$

where d is a cut-off parameters assumed to lie between the second- and third-neighbors, the value of d is$a < d < \sqrt{2}a$, a is a lattice constant. For Fe element, the expression of $\Phi(r)$ can be modified by

$$\Phi(r) = (r-d)^2 + \frac{\beta}{d}(r-d)^3, \tag{4}$$

where the range of these parameters should be set to enable the $\Phi(r)$ reaching the maximum in first- nearest-neighbor. For example, if $d = a$, then $\beta < 4.975$; otherwise, $d = \sqrt{2}a$, then $\beta < 1.7199$.

In Eq. (1), $V(r)$ is a repulsive two-body interaction, interpreted in the tight-binding theory as the repulsion between core electrons on neighboring atoms, expressed as

$$V(r) = \begin{cases} (r-c)^2(c_0 + c_1 r + c_2 r^2) & r \leqslant c \\ 0 & r > c \end{cases} \tag{5}$$

where c is a cut-off parameter, just like the parameter d; c_0, c_1, and c_2 are free parameters fitting to experimental data based on specific elements. All parameters of FS potentials for Fe have been listed in Table 1.

2.2. Transformation for potential energy surface

Actually, the potential function of a cluster corresponds to a complicated potential energy surface in hyperspace. The potential energy surface describes the relationship between the cluster energy and the relative position of each atom in the cluster. Therefore, investigating the stable structure of a cluster by minimizing its total energy is to search the global minimum of the potential energy surface. However, it is difficult to find the lowest energy on the potential energy surface directly even for a system consisting a few atoms due to the complexity of potential energy surface. To reduce the search space and improve the searching efficiency, in this work we transform the potential energy surface into many less-intricate basins by employing a local minimization for the structures [24].

Since the potential energy surface is a curve in the multi-dimensional space, it is impossible to directly depict the surface. Here, we display the transformation diagram of the potential energy surface in two-dimensional surface in Fig. 1. We may transform the complicated potential energy surface into less-intricate basins by local minimization procedure. The transformation not only avoids the unstable transition state on potential energy surface, but also decreases the energy barrier. It makes the system freely go through the basin boundaries of potential energy, therefore simplifies the optimization process.

2.3. Cluster-based niching differential evolution algorithm

2.3.1. Structural optimization of a cluster

The structural optimization of a cluster can be described as follows. For a cluster consisting of N atoms, the total energy of all atoms is defined as its potential energy. When the potential energy reaches its minimum, the search target is the atom coordinates in the three-dimensional space.

The objective function of the structural optimization is the potential energy according to Eq. (1). It can be described as

$$\min f = \min E_{tot}(R) \tag{6}$$

where E_{tot} is the potential energy of a system, R represents the atomic distance matrix, and is given by

$$R = \begin{bmatrix} r_{11} & \cdots & r_{1N} \\ \vdots & \ddots & \vdots \\ r_{N1} & \cdots & r_{NN} \end{bmatrix} \tag{7}$$

$$r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \tag{8}$$

x_i, y_i, and z_i denote the coordinates of atom i in three-dimensional space. Since the interatomic distance is relative, it means $r_{ij} = r_{ji}$. Therefore, the distance matrix R is a symmetric matrix, and the diagonal values are zero because the distance between an atom and itself is zero ($r_{ii} = 0$).To make the general multi-populations differential evolution algorithm more effectively during the structural optimization of cluster, in the base of primal algorithms [25,26], we have proposed a cluster-based niching differential evolution algorithm by combining the cluster pool, the niche method, and the differential evolution algorithm instance, as shown in Fig. 2.

2.3.2. Cluster pool

Essentially, the cluster pool is a collection of many different clusters (individuals) with the same atomic number. The cluster pool is used to keep the individual diversity during structural optimization of clusters. Moreover, it is a great solution for clustering and distinguishing the clusters. The initialization, clustering, and update of the cluster pool play a significant role in the whole algorithm. The three procedures have been described in detail below.

2.3.2.1. Initialization of cluster pool. Consider a cluster consisting of N atoms, the atom coordinates are represented by three dimensional