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基于结构聚类的小生境差分进化算法的Fe团簇结构优化研究

Research on Optimization of Fe Clusters Structure Based on Structural Clustering Niche Differential Evolution Algorithm

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摘　要

团簇被称之为“物质第五态”。它是材料科学的新起点，在许多领域都有着广泛的应用。团簇的稳态结构对其独特的物理和化学等性质起到了至关重要的作用，因而受到许多学者的广泛关注。由于团簇的大小在几埃到几百埃之间，尺寸非常小，用实验设备很难合成和直接观测。因此用理论研究的方法来探究团簇的稳态结构显得十分重要。但是寻找团簇的稳态结构十分困难，除了基态结构之外，还存在成千上万的亚稳态结构。目前团簇优化问题已被学者证明为NP难问题，因此用传统的优化方法难以获得最优解，于是使得基于进化算法的全局优化方法得到了广泛应用。

本文以Fe团簇作为研究对象，采用Finnis-Sinclair势来描述原子间的相互作用，以能量最小值为优化目标，使用基于团簇结构聚类的小生境差分进化算法，对目标函数进行求解。该算法包含团簇池和差分进化算法实例两部分。团簇池负责小生境子种群的生成，使用团簇的结构特性作为分类标准，将结构相似的团簇进行聚类，产生小生境子种群。差分进化算法实例负责种群的进化，针对团簇优化问题采用多种变异策略，使用面切的交叉方式，添加了调整策略，使得算法更加适合于团簇结构优化。

本文实验分析了团簇池大小对算法收敛速度和结构多样性上的影响：团簇池越大，算法结构多样性就越高，但是其收敛速度就越慢。同时，本文从能量变化和结构演变的角度验证了算法的有效性。另外，本文采用平均结合能、二阶差分能、剩余能、平均近邻原子距离和平均配位数等指标分析了Fe团簇的结构稳定性，验证了算法的稳定性。实验结果表明：本文提出的算法用于求解Fe团簇结构优化问题是有效且稳定的。

关键词：Fe团簇；稳定结构；结构聚类；小生境；差分进化算法

Abstract

The cluster is known as the material fifth state. It has been widely used in many fields, such as physics, chemistry, biology, and engineering. And the cluster is regarded as the new start of the material science. The stable structures of clusters have attracted increasing attention because they play a vital role in their unique physical and chemical properties. The size of cluster is ranged from several angstroms to several hundred angstroms. It is too small to be compounded or observed by experimental equipment. Therefore, it is more important to investigate the stable structures by theoretical research. To search the best stable structure of clusters is very difficult because there are thousands of meta-stable structures during the reaching process, except the ground structures. Structural optimization of clusters is a NP-hard problem, which has been proved by scholars. However, the traditional optimization methods are unable to solve this NP-hard problem. Thus, the evolutionary algorithm has been widely used in structural optimization of clusters.

In this paper, we focus on structural optimization of Fe clusters, with the Finnis-Sinclair potential employing to describe the interaction between atoms. The objective of the optimization problem is to minimize the energy of the Finnis-Sinclair potential. The differential evolution algorithm based on structural clustering niche is proposed to solving the optimization problem. The algorithm contains the cluster pool and the differential evolution algorithm instance. The cluster pool is responsible for generation the niche sub populations. The clusters can be classified with structure characteristics of the clusters as the classifying criterion. By clustering the clusters with similar structures, the niche sub populations can be generated. The differential evolutionary algorithm instance is responsible for the evolution of the population. For the structural optimization of clusters, 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 structure optimization of clusters. In the experimental part, the performance of the algorithm has been analyzed by discussion the pool size effect on the convergence speed and structural diversity. The experimental results show that the larger the clusters pool size is, the higher the structural diversity is. However, the convergence speed of the algorithm is slower. Meanwhile, the accuracy and effectiveness of our algorithm has been verified from the points of the energy evolution and structure evolution. In addition, the structural stability of the Fe clusters have been analyzed by calculating the average binding energies, the second differences energies, the excess energies, the average neighbor distances and the average coordination numbers. All the experimental results show that the proposed algorithm is effective and stable for the structural optimization of Fe clusters.

Keywords: Fe clusters; Stable structure; Structure cluster; Niche; Differential evolution algorithm;

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