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Global minima of iron clusters described by Gupta potential

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Abstract

In this paper, we present global minimum energy for iron clusters, ranging from sizes $N=2$ to 100 atoms, described by the phenomenological Gupta potential. Our optimized structures and symmetry groups are in agreement with previous ones obtained using Finnis–Sinclair potential; but our energy levels and nearest neighbor distances differ slightly. The origins of the differences are related back to the differences in the potentials.

Keywords: Iron clusters; Gupta potential; Global optimization

1. Introduction

The behavior and characteristics of condensed matter systems are controlled by their structure, since mechanical, transport, optical, chemical land magnetic properties are determined by them. Thus, establishing the way, the constituent atoms arrange spatially to form molecules, nanoclusters and crystals, is the fundamental problem of solid state physics [1]. Nanoclusters are aggregates that contain up to million atoms and constitute the building blocks of nanoscience; the structure of transition metal nanoclusters (with diameters between 1 and 10 nm) is of significant theoretical and practical interest due to their potential use in ultrahigh density magnetic recording materials [2], catalytic particles in the synthesis of carbon nanotubes [3,4] and other applications in electronics and optics. Due to their small size, nanoclusters can remain in a "liquid-like" state at temperatures well below the bulk melting point [5,6], and their magnetic moments can exceed bulk value up to cluster sizes of several hundred atoms [7]. In general, the geometric structures of the clusters do not resemble those of the bulk metals since there are no constraints on rotational symmetry from the crystallographic restriction theorem. The structure of an iron cluster is one of its most important properties, yet it is a property that can be hard to access for clusters.

Computer simulations are carried out in the hope of understanding the properties of assemblies of molecules in terms of their structure and the microscopic interactions between them.

This serves as a complement to conventional experiments, usually leading only to an indirect measurement of the structure; consequently, experimental results need to be compared to what would be expected for candidate structures. The experimental procedures have been successful isolating the larger species of fullerenes and

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determining their geometries. However, sophisticated global minimization techniques have been developed and implemented in order to find the lowest energy configuration among a huge number of local minima [1,8–10]. Given the complexity of the problem (for example, the potential energy surface of 13 atom Lennard–Jones cluster has about a thousand of minima [10]), it is not surprising that some degree of controversy and uncertainty are always present. The ground state structure of small clusters is still not known with certainty and many isomers structure have been proposed.

The lowest energy structure of cluster can be determined using ab-initio electronic structure methods. But when the number of atoms constituent the cluster becomes high, ab-initio calculations which are very time consuming. Therefore, several semi-empirical potentials [11–13] which describe correctly the interactions amongst cluster atoms, have been developed. For accurate determination of energy, the potential must incorporate: well modeled different external surfaces, twin planes, different crystal structures, and the response to strain. To model the potential temperature dependence of the structure, vibrational properties need also to be well described [14]. Therefore, prediction of the correct structure of a cluster represents a tough challenge for a potential in use. Furthermore, it is often not clear which of the available potentials will work better for a considered system. Even using some semi-empirical potentials to determine the minimal configurations of structures, the convergence is not always guaranteed particularly when the number of atoms constituent the structure becomes high.

The objectives of this study are to use the phenomenological many-body Gupta potential to determine the lowest energy structure of all Fe_N clusters in the range $2 \leq N \leq 100$. Thereafter we compare our results with those obtained using Finnis–Sinclair (SE-MO and Lennard–Jones) [15] potentials. The most important fact in the Gupta potential is that for a sufficiently long time, it converges directly toward the optimized structure and this occurs whatever be the initial configuration. Consequently, this method can allow one to simulate systems much larger than previously accessible, widening the range of materials science issues that can be addressed. Gupta potential allows one to perform simulations involving up to three hundred of atoms on small work stations. This type of potential has been extensively used in metallic cluster simulations [16,17], and it leads to results that are in good agreement with those generated from first-principles methods [18]. We work in a similar spirit as Refs. [12,14,19], where possible structural patterns for sodium, aluminum, zinc and cadmium clusters modeled by the Gupta potential have been suggested.

The paper is organized as follows: In Section 2, we describe the model potential and provide details on the simulation method. In Section 3, total energy behavior and some of the global minimum cluster structures obtained from our calculations are presented and compared with those obtained using FS potentials and SE-MO theory. A summary of this work is presented in Section 4.

2. Potential and methodology

2.1. Potential description

The many-body model potential used in this work is the semi-empirical Gupta potential [20–22] which was derived from Gupta's expression for cohesive energy of bulk material [21] and is based on the second moment approximation of a tight-binding Hamiltonian [21]. The interaction between the iron atoms in the long distance was disregarded. The cohesive energy of the system depends on five parameters, and is written in terms of repulsive pair and attractive many body terms which are obtained by summation over all atoms and it is expressed by the summation of the total bonding energy between two atoms as follows:

$$E = A\sum_{i=1}^{N}\sum_{j>i}^{N} e^{p\left(1-\frac{r_{ij}}{r_0}\right)} - \xi\sum_{i=1}^{N}\sqrt{\sum_{i=1}^{N} e^{2q\left(1-\frac{r_{ij}}{r_0}\right)}} \qquad (1)$$

where r_{ij} is the interatomic distance between atoms i and j; r_0, A, ξ, p and q are adjustable parameters that represent, respectively, the equilibrium Fe–Fe bond, the repulsive coefficient, the attractive coefficient, and the last two denote the range of the interaction [21]. The parameters of the Gupta potential that we used are shown in Table 1.

2.2. Methodology

All the global optimization calculations in the work were performed using a numerical code based on the constant-energy molecular dynamics method. We have calculated the structural changes as a function of the cluster energy. Within this method, Newton's equations of motion are solved for each atom within the cluster using

Table 1
Gupta parameters for iron cluster.

$A = 9.6000$ eV	$p = 4.5000$	$\xi = 1.8000$ eV	$q = 0.4000$