J. At. Mol. Sci.
doi: 10.4208/jams.102312.112412a

Vol. **4** , No. 3 , pp. 235-244
August 2013

Structural properties of Rh_n ($n = 2 \sim 100$) clusters by using Gupta potential with the simulation of quenching method

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Received 23 October 2012; Accepted (in revised version) 24 November 2012
Published Online 28 June 2013

Abstract. The ground-state geometries and energies of $Rh_n (n = 2 \sim 100)$ clusters are investigated by using Gupta potential combined with the molecular dynamics simulated quenching method and the genetic algorithm. Our results show that: As comparing the lowest energy structure obtained from the simulated quenching method which can be regarded as the ground-state structure, almost all these ground-state geometries can be found (except Rh_{50}) by using the genetic algorithm for clusters containing 60 or less atoms, but the efficiency of capturing the ground-state geometry decreases obviously with increasing the cluster size. The effective temperature range for obtaining the ground-state energy (geometry) is obtained by systematically analyzing the energy distributions of the simulated quenching structures, and the correlation between the quenching method of finding the ground-state and the cluster size is also investigated further.

PACS: 36.40.-c, 32.10.-f, 31.15.-p, 61.46.Bc

Key words: Gupta potential, cluster, ground-state, molecular dynamics, simulated quenching

1 Introduction

Clusters are aggregates composed of several to thousands of atoms (molecules) bonding in certain physical or chemical forces, that exist stably in microscopic state [1]. It has been aroused a great interest, just because of its unique physical and chemical properties and applications in nano-electronics, nano-catalyst and new material physics [2-8]. It has already become a new and significantly important field to study the formation, structures, evolution behavior and other properties of clusters. As the first step, determination of the ground-state geometry of a cluster plays a significant role in studying many other

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properties of the cluster. For free clusters containing three or more atoms, their geometrical structures can not be measured directly from experiments so far, and it becomes very important to ascertain the ground-state of clusters combining with theoretical calculations. Nowadays theoretical computations are mainly based on either the first-principles (ab-initio) calculations in quantum mechanics level or the empirical (semi-empirical) calculations based on interatomic potentials. The former has a very accurate result, but large amount of calculation time needed, and it is very difficult to handle a cluster with relatively large size (especially more than 20 atoms). The latter, according to the different ways of simulation, can be classified into several methods such as the molecular dynamic method [9,10] the Monte Carlo simulation method [11,12] the genetic algorithm [13-15], the simulated annealing method [16,17] and the simulated quenching method, etc.

As a transition metal and constituent of many catalysts, rhodium plays important role in catalytic field, and particular attention has been paid to studying rhodium clusters. Chien and co-workers[18] studied the paramagnetic and ferromagnetic properties of Rh_n(n=2∼58) clusters based on the generalized gradient approximation (GAA) within the density functional theory (DFT); Aguilera-Granja and co-workers [19], by using the genetic algorithm combined with self-consistent spd tight binding method, systematically studied the structural and magnetic properties of Rh_n (n=4∼26) clusters; Zhang and co-workers [20] profoundly studied the ground state structures of Rh_n and Pt_n (n=2∼20) clusters by applying the genetic algorithm. Many researchers use the traditional genetic algorithm and Monte Carlo simulation method to solve the ground-state structures (energies) of clusters containing less than 60 atoms, but the solving methods are still so complex as increasing the cluster size.

In this paper, not only we systematically studied, by using the molecular dynamic method based on the semi-empirical Gupta interatomic potential combined with the molecular dynamic simulation of quenching technique, the ground-state structures (energies) of Rh_n (n=2∼100) clusters, but also analyzed the contrast of the genetic algorithm results.

2 Computational methods

The interaction between atoms, which is depicted by the potential function, is the fundamental to determine the dynamic behaviors of clusters. In this letter, the interaction between atoms of Rh clusters are described by using the semi-empirical many body Gupta potential [21] based on the embedded-atom potential and tight-binding model of the second moment approximation, in which the potential parameters are obtained from fitting the relevant physical parameters of crystal (cohesive energy, lattice constant and elastic moduli, etc). Moreover, this kind of many body potential has been extensively used to study the geometries [22] and dynamic behaviors [23] of the metal and alloy clusters. Gupta potential can be written as the sum of a Born-Mayer type repulsive part and a