

## Effect of the Equilibrium Pair Separation on Cluster Structures

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**Abstract.** The effect of the equilibrium pair separation on the evolution of cluster structures is investigated based on a new proposed pair potential. The computational results demonstrate that the potential with large equilibrium pair separation stabilizes decahedra and close-packed structures, while disordered structures appear for the potential with small equilibrium pair separation. The icosahedral clusters are dominated in the middle range of equilibrium pair separation. For the small size clusters ( $N \leq 24$ ) the dominated structural motif is the polytetrahedra, which is almost independent of the details of the potential.

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### 1 Introduction

Understanding the cluster structure represents one of the crucial issues in nanoscience. Exploring the novel structure of nanoclusters has brought a big challenge to traditional method and technique used widely for bulk condensed matters [1]. Up to date, few direct measurements of cluster structures are available experimentally [2], and much of the current theoretical understanding of cluster structures has been derived from atomic-scale molecular-dynamics (MD) and Monte Carlo (MC) simulations [3].

The computer simulations have been carried out on various systems. The model clusters, described by Lennard-Jones (LJ) and Morse potentials, have been studied extensively (e.g., [3]). Metal clusters are also widely studied using both density functional

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theory and classical many-body potentials (e.g., [3,5,6]). A few studies have extended to large molecule systems [7–17] and multi-element systems [18–26]. Over the past decades, many exotic structures, which are probably forbidden in bulk materials, have been reported. The excellent examples include the cage structures of carbon [27], the Icosahedral (IH) [28,29] and decahedral (DH) [30,31] atomic shell structures of metals, and the recent found cage structures of gold [32,33].

Many papers have reported the general structural effects of the different contributions to the interaction. For example, Doye and Wales found that the Friedel type oscillation in atomic potentials can strongly modulate the cluster structures [34–36]. The effect of the potential shape on the nature of disordered structure are also studied [37,38]. Baletto *et al.* have investigated crossover between different structural motifs (icosahedra, decahedra, and octahedra) for a few many-body potentials [39,40]. Doye and Wales investigated the structural evolution for a set of Sutton-Chen families of potentials [41]. Gong and his coworkers have studied the relativistic effect on the structure of gold clusters, which leads to the finding of cage-like structures [32,33].

Since the shape of simple pair potential could be adjusted in a comprehensive way, pair potentials provide intuitive understanding of the general effects, *i.e.*, the effect of potential shapes on cluster structures. Previously, the effect of the potential range and anisotropy on the cluster structures were studied for many simple pair potentials. Braier *et al.* have investigated six- and seven-atom Morse clusters over different interaction range [42]. A similar study was carried out on other model potentials [43,44]. Doye and Wales have made systematic studies on how the structure of Morse clusters changing with the interaction range. They found that the decrease of the interaction range results in destabilizing strained structures [7,45–48].

Although substantial efforts have been made by many researchers, the knowledge about the relationship between cluster structure and potential shape is still limited. The further studies along this line are needed. In this paper, the issue about how the equilibrium pair separation ( $d_{EPS}$ ) affecting the cluster structure is studied. Physically, changing  $d_{EPS}$  corresponds to changing the effective size of atoms/molecules. The importance of the atomic/molecular size has been shown in recent studies on  $C_{60}$  [49]. Our current studies will shed light on the general effect of the equilibrium pair separation on the cluster structures.

The remainder of the paper is organized as follows. The following section describes the new model potential and the computational details. The cluster structures for a few selected parameters are presented in Section 3. The conclusions drawn from this work are summarized in Section 4.

## 2 Computational details

The potential we proposed is originally prompted by the effective pair potential [50] of many-body potential for iron [51,52], then we parameterize it into the current form: