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COPPER CLUSTERS: STUDY OF GEOMETRIC STRUCTURE USING COMPUTER SIMULATION

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COPPER CLUSTERS: STUDY OF GEOMETRIC STRUCTURE USING COMPUTER SIMULATION

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Abstract

In this work, we investigated the geometric structure of small neutral copper clusters with low energy using the MD (Molecular Dynamics) method. When calculating the processes of interatomic interaction, we used a potential EAM (Embedded-atom method). A computer model of Cu_n (n = 2-13) clusters has been created. The geometric shapes of the Cu_2, Cu_3, Cu_4, Cu_5, Cu_6, Cu_7, Cu_8, Cu_9, Cu_{10}, Cu_{11}, Cu_{12}, and Cu_{13} clusters have been studied and the structural parameters (Cu-Cu bond distance) have been calculated. The results obtained in the computer model were compared with the experimental results.

Keywords: *Copper clusters, Molecular Dynamics, Embedded-atom method, Low-atomic, low-energy*

Introduction. It is difficult to imagine modern science without the use of computer modeling. Modification of the mathematical model of the original object makes it possible to determine its properties relatively quickly and at the lowest cost. The study of objects using computer simulation, in contrast to a purely theoretical approach, allows you to study them in their characteristic state. Currently, experiments in solid state physics are expensive, but it is possible to test a model that replaces a real object by simulating scientific research using modern computers [1].

Due to the widespread use of metal clusters in the field of nanotechnology, experimental and theoretical studies of clusters are currently undergoing significant development. As a result, there is growing interest in the use of computer modeling in addition to experimental methods to create and study the factors that determine the morphology of low-atomic clusters. Clusters are nano-sized aggregates that are very different from solid materials [2].

In this paper, we consider the modeling of low-atomic copper-metal clusters, as well as the geometric arrangement of atoms in these clusters.

Currently, many methods have been developed to study the process of modeling the behavior of nanoclusters. They are discussed in section 2 of the article. The results and discussions are presented in section 3, and the conclusion - in section 4.

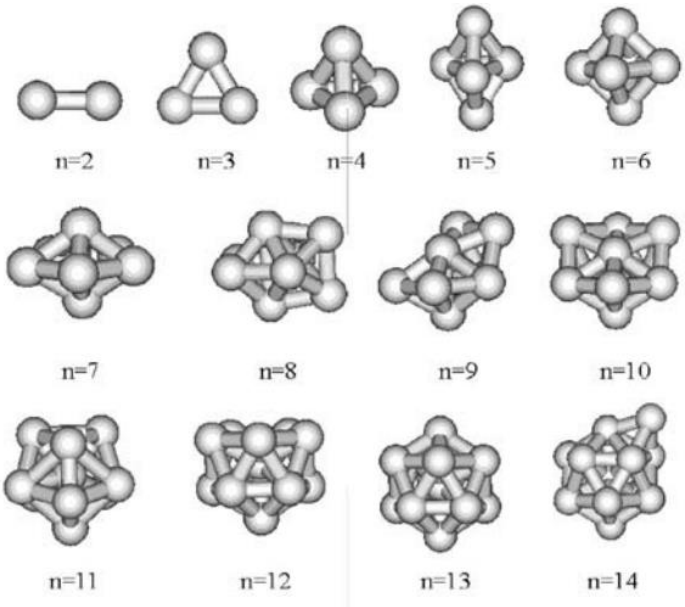

Figure 1. Low-atomic and low-energy copper clusters (Cu_n, n = 2-14) [2].

[2] shows the structures of copper clusters of different sizes and low energies. We have placed some of them in Figure 1.

Figure 2. Main structure of states of Cu_{11}, Cu_{12} and Cu_{13} clusters. [9]

In [9], the results of various symmetries, binding energies, and relative stability for the study of Cun clusters ($n \leq 24$) are presented.

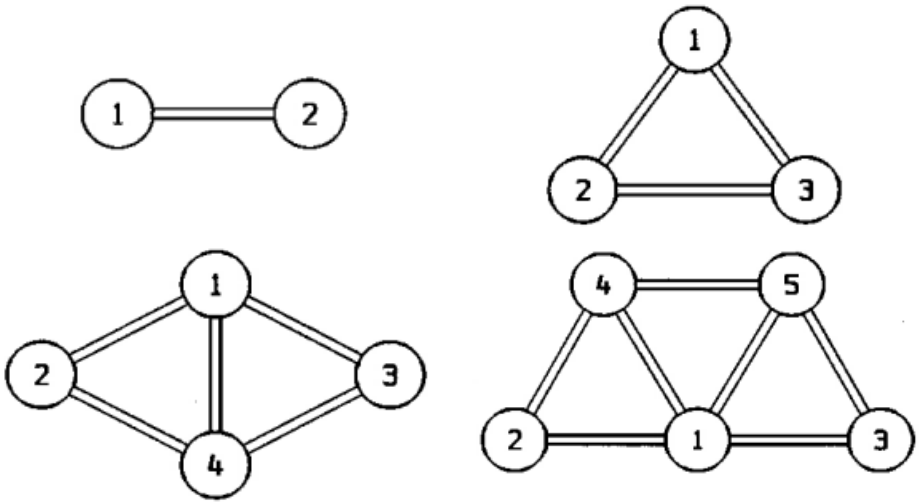

Figure 3. Neutral copper clusters (Cu_n, n = 2-5) [8].

In [8], the structure and stability of neutral and ionic low-atomic (up to ten atoms) copper clusters were determined using density functional calculations.

[10] discussed a number of features associated with the geometry of low-atomic (up to 10 atoms) copper clusters and compare them with the results available in the literature.

Theoretical research methodology. At present, the MD method and its analogs are increasingly used for atomistic modeling. The main reason for this is that this method is responsive to real-time simulations. Therefore, we believe that the MD method gives sufficient results for atomistic modeling.

The MD method is based on solving the system of equations of Newton's second law for all atoms that make up the system being modeled. The upper limit of the number of atoms included in the modeled object or in the simulation cell when using periodic boundary conditions increases with the expansion of the capabilities of computer technology.

There are two main types of MD (adiabatic and isothermal). The adiabatic type is more suitable for classical mechanics and is the result of the fact that the total energy of the simulated system does not change. However, this version is rarely used because it does not take into account energy consumption, which is usually less consistent with the development of real systems. In isothermal MDs, the mechanical algorithm is supplemented by a special algorithm (a thermostat that maintains a given temperature). First, such an algorithm must fulfill its main task. Secondly, it should not react to significant interference in the phase trajectory of the system, i.e., in order not to distort the scenario of its evolution, prescribed by the system of equations of Newton's second law:

$$\begin{aligned} a_{xi} &= \frac{dv_{xi}}{dt} = m^{-1}\left(\Sigma_{i\neq j}F_{xij} + \Sigma_i f_{xi}\right) \\ a_{yi} &= \frac{dv_{yi}}{dt} = m^{-1}\left(\Sigma_{i\neq j}F_{yij} + \Sigma_i f_{yi}\right) \\ a_{zi} &= \frac{dv_{zi}}{dt} = m^{-1}\left(\Sigma_{i\neq j}F_{zij} + \Sigma_i f_{zi}\right) \end{aligned} \quad (3)$$

where a_{xi} , a_{yi} , a_{zi} are the components of the acceleration vector of the "i-th" atom, v_{xi} , v_{yi} и v_{zi} – velocity vector components, t – time, m – mass of an atom, F_{xij} , F_{yij} и F_{zij} – components of internal forces, acting on atom i , a f_{xi} , f_{yi} и f_{zi} – components of external forces, equal to zero for a free nanoparticle [3].

The level of accuracy of the results obtained using such algorithms is very high. Software, on the other hand, is more complex and requires a lot of memory to store a large number of values.

Based on the above relationship, in practice, the more convenient Verlet algorithm is widely used [4]:

$$\vec{r}(t+\Delta t) = 2\vec{r}(t) - \vec{r}(t-\Delta t) + \vec{a}(t)(\Delta t)^2,$$

$$\vec{v}(t) = \frac{\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)}{2\Delta t}$$

Simulation details. When modeling metallic systems, multiparticle potentials are used that correspond to the "Embedded atom method" [5].

Based on the above, we used the LAMMPS software package [11] developed by Sandia National Laboratories to model the geometric structure of silver clusters by the MD method [6,7]. When calculating the processes of interatomic interactions, we used the potential EAM (Embedded Atomic Method) [5]. We used the Jmol program [12] to visualize the geometric structures of low-atomic copper clusters.

In each simulation, after creating the initial configuration, we minimized the fall below 10000 steps. The Verlet algorithm was used to integrate Newton's equations of motion with a time step of 0.0001 ps. The length of each simulated trajectory was 1000 ps (1 ns).

Analysis and results. Figure 4 shows the geometric structures of small atomic copper clusters. In these pictures, the balls represent copper atoms, the brown lines between the balls show the interaction between the atoms.

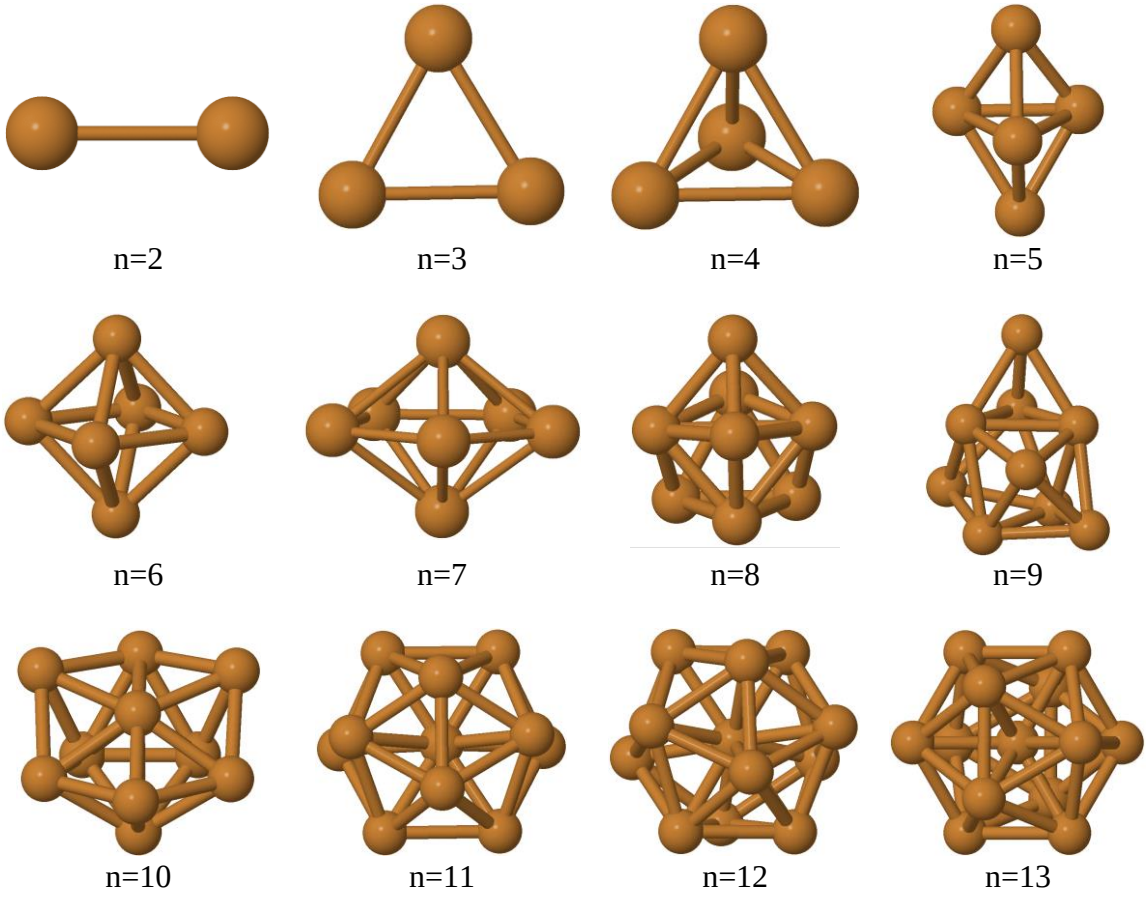

Figure 4. Geometric structures of neutral copper clusters for n = 2-13.

The Cu_2 cluster has a cross-sectional shape connecting two points. The Cu_3 cluster has the shape of an equilateral triangle. Cu_4 has the shape of a regular triangular pyramid. The Cu_5 cluster consists of five atoms, three of which are in one plane, and the other two atoms are symmetrically above and below the center of this rectangle. The Cu_6 cluster consists of six atoms, of which 4 atoms are in the same plane, and the other two atoms are located symmetrically above and below the center of this rectangle. The Cu_7 cluster consists of seven atoms, of which 5 atoms are in the same plane, and the other two atoms are located symmetrically above and below the center of this pentagon. The Cu_8 cluster forms 4 atoms and a simple parallelogram in one plane, the remaining one atom is above the center of the parallelogram, and the other three atoms are below the center of the parallelogram. As can be seen from Figure 2, the shape of the clusters from Cu_9 to Cu_{12} has an unusual geometric shape, approaching the shape of a sphere. The Cu_{13} cluster has a spherical shape.

Table-1. Comparative table of structural parameters (Cu-Cu bond distance) of neutral copper clusters up to ten atoms (values are in Å**).**

Cluster	Structure parameters		
	Reference [8]	Reference [9]	This work
Cu_2	2.21		2.16
Cu_3	2.30	2.25	2.28
		2.24	2.28
		2.24	2.28
Cu_4	2.35	2.23	2.35
	2.32	2.22	2.35
		2.24	2.35
Cu_5	2.30	2.23	2.36
	2.42	2.38	2.42
Cu_6	2.36	2.4	2.36
	2.47	2.39	2.38
	2.42	2.41	2.41
	2.28		2.57
Cu_7	2.39	2.41	2.39
	2.39	2.63	2.42
		2.45	2.39
Cu_8	2.35 2.47	2.41	2.41 2.42
	2.38 3.07	2.61	2.41 3.12
	2.39 2.38	2.59	2.42 2.39
	2.35 2.47	2.39	2.39 2.42
Cu_9	2.44 2.40	2.44	2.42 2.41
	2.41 2.37	2.59	2.42 2.41
	2.44 2.37	2.41	2.42 2.41
	2.43 2.38		2.42 2.41
Cu_{10}	2.33		2.39
	2.42		2.44
	2.45		2.46

Conclusion. We investigated the geometric structure of small neutral copper clusters using the EAM potential in the MD method. Our geometric results showed good compatibility with experimental and other theoretical studies. The general trend we found is that copper clusters with the same number of atoms are more stable than odd copper clusters.

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References

1. Rasulov A.M., Ibroximov N.I. (2019). Clusters Deposition on Surface an Atomic Scale Study by Computer Simulation Method. Journal of App. Math. And Phys., 7, 2303-2314.
2. Böyükata M., Belchior J.C. (2008). Structural and energetic analysis of copper clusters: MD study of Cu_n (n = 2-45). J. Braz. Chem. Soc., Vol. 19, No. 5, 884-893.
3. Talizin I.V. (2019). Molekulyarno-dinamicheskoe issledovanie termodinamicheskix i kineticheskix aspektov plavleniya i kristallizatsii metallicheskix nanochastits. S.36-39.
4. Allen M.P., Tildesley D.J. (2017). Computer Simulation of Liquids. Published to Oxford Scholarship, S. 78-82.
5. Murray S. Daw., Baskes M.I. (1984). Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. J. Phy. Rev., Vol 29, No 12, 6443-6453.
6. Bogatikov E.V., Bityutskaya L.A., Shebanov A.N. (2013). Modelirovanie nanoklasterov metodom molekulyarnoy dinamiki. Izdatelsko-poligraficheskiy tsentr Voronejskogo gosudarstvennogo universiteta, S.10-24.
7. Michael P. Allen. (2004). Introduction to Molecular Dynamics Simulation. Computational Soft Matter, John von Neumann Institute for Computing, NIC series Vol. 23, pp. 1-28.
8. Jug K., Zimmermann B. (2002). Structure and stability of small copper clusters. J. Chem. Phy., Vol 116, No 11.
9. Kabir M., Mookerjee A., Bhattacharya A.K. (2004). Copper clusters: electronic effect dominates over geometric effect. Eur. Phys. J. D 31, 477-485.
10. Li Ch.G., Shen Zi.G., Hu Y.F., Tang Ya.N., Chen W.G., Ren B.Z. (2017). Insights into the structures and electronic properties of Cu_{n+1}^{μ} and Cu_nS^{μ} (n=1-12; μ=0, ±1) clusters. Scientific Reports 7 (1).
11. https://docs.lammps.org/Manual.html
12. https://chemapps.stolaf.edu/jmol/docs/