# Study of Electronic Properties of Copper Nanoclusters

Seifollah Jalili and Laya Sabouhi
Department of Chemistry, K. N. Toosi University of Technology, P.O. Box 15875-4416, Tehran, Iran
Department of Chemistry, Payame-Noor University of Ardakan, Yazd, Iran
Emails:sjalili@kntu.ac.ir, lsabouhi@sina.kntu.ac.ir

## Introduction

Small metallic clusters are an interesting group of compounds in physical chemistry and solid state physics that have many applications in different fields. An important feature of these compounds is that it is possible to control their properties via their size. Changing the dimension of these clusters can create desirable effects. In this paper we have used quantum mechanical calculations to study copper clusters. The effect of oxygen adsorption on the electronic properties of these clusters is studied using energy and density of states (DOS) calculations.

Keywords: Copper clusters, Electronic structure, Oxygen adsorption, Density of States (DOS), Density Functional Theory (DFT)

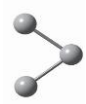
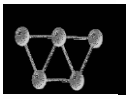
## Computational Details

All calculations were performed using GAUSSIAN 98 program. Six different $Cu_n$ clusters with $2 \leq n \leq 8$ were considered. The geometry of these clusters was optimized using B3LYP/LANL2DZ level of theory. Density of states was calculated and plotted using Gauss Sum 1.0.5 code.

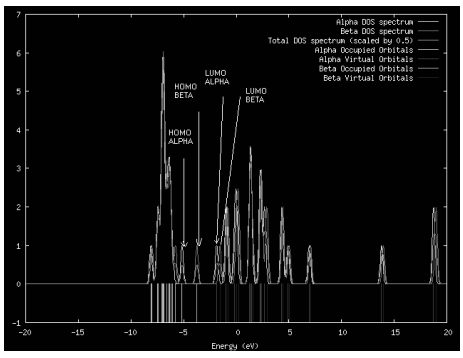
## Results and Discussion

Energy values for optimized clusters are shown in Table 1. According to these data, the energy decreases with increasing cluster size. The smaller clusters are very unstable and this is one of the problems in the small cluster synthesis. The clusters' energy gaps are also shown in Table 1. The values of these gaps are all in the range corresponding to metals (i.e. less than 1 eV). In cases with spin multiplicity, two values are obtained for spin up and spin down electrons.

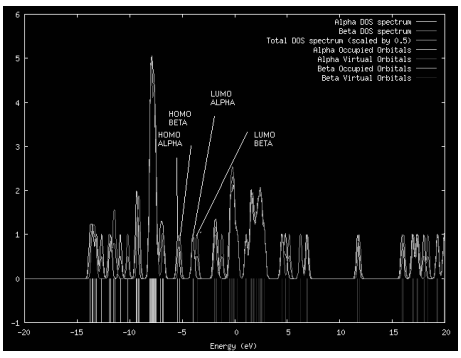
Table 1. Energy values, spin multiplicity and energy gap for some optimized clusters.

| # atoms | structure | energy (hartree) | spin multiplicity | energy gap (eV) |
|---|---|---|---|---|
| 2 |  | –392.307 | 1 | 0.125 |
| 3 |  | –588.460 | 2 | 0.148 (a)<br>0.726 (þ) |
| 4 |  | –784.659 | 1 | 0.069 |
| 5 |  | –980.841 | 2 | 0.088 (a)<br>0.083 (þ) |
| 6 |  | –980.841 | 1 | 0.071 |
| 7 |  | –1373.152 | 2 | 0.057 (a)<br>0.120 (þ) |
| 8 |  | –1569.361 | 1 | 0.084 |

Adsorption of oxygen molecule decreases the energy of all clusters, and therefore makes them stable. This stability is completely acceptable, because the Cu atoms have $4s^{1}3d^{10}$ configuration and tend to lose one electron to become stable. This electron is transferred to adsorbed oxygen atoms and increases the stability by at least 200 hartrees. Fig. 1 shows the density of states for triatomic cluster before and after oxygen adsorption. The DOS plots show that, the conductivity increases. The electron transfer occurs easily because of small energy gap.




(a)




(b)

Figure 1. DOS plots for triatomic copper cluster before (a) and after (b) oxygen adsorption.

References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