IONIZATION POTENTIALS OF FE MICROCLUSTERS

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ABSTRACT. Ionization potentials of small iron clusters have been obtained within the local spin-density approximation and model "atom in jellium". The nonmonotonic character of the size-dependence of an ionization energy with a cluster size has been shown.

1. INTRODUCTION

In recent year size-selective chemical and physical properties of small metal clusters (SMC) have attracted great attention. This interest is bound up with the effective use of microclusters in technological processes including a geterogeneous catalysis. SMC are excellent catalysts and it is well known that the activity and selectivity of such catalysts depend on the cluster size. Recently the strong correlation between the chemisorption reactivity of free SMC and their ionization energy has been shown [1].

We have made an attempt to study the size dependence of an ionization potential (IP) of spherical Fe-clusters containing up to twenty atoms. The IP of these atomic systems has been experimentally obtained by authors of [1-3].

2. RESULTS AND DISCUSSION

In the calculations we simulated atoms of a Fe cluster by Fe

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atoms embedded in the centre of the spherical-finite jellium of a various size. The jellium sphere radius R is defined by the short cut between the atom and the cluster surface.

IP of "atom in jellium" was obtained using the ground-state theory (the local spin-density approximation) by the self- consistent calculation and subtraction of total energies of the neutral and ionic ground states.

It was found that ionization thresholds of atoms of the Fe cluster are different and depend on positions of the atoms in relation to the cluster surface. The IP of the cluster

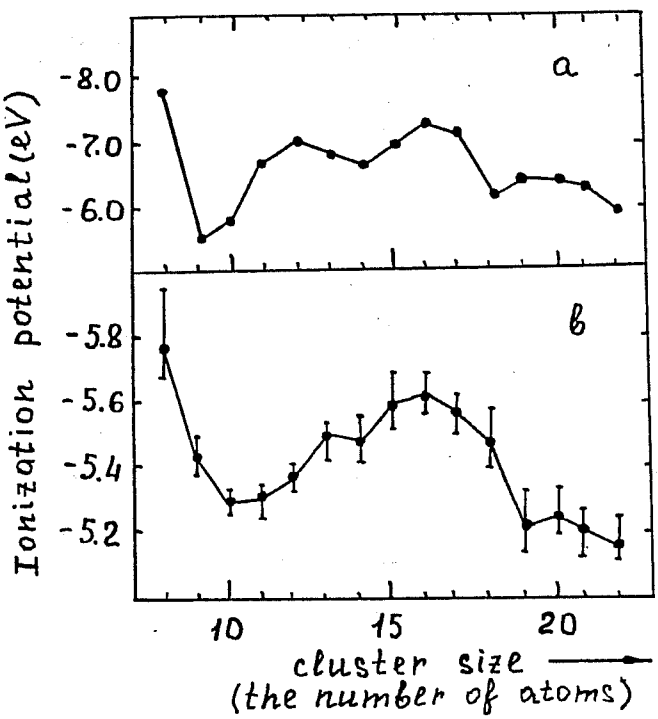

Figure 1. The size dependence of ionization potentials of iron clusters: theory (present work) (a) and experiment [1] (b).

atom having the least ionization energy of all was chosen as that of the Fe cluster.

IPs of Fe clusters with BCC and FCC geometry structures (cluster atoms are placed around the central atom like BCC or FCC coordination spheres of bulk iron) have been calculated. IP was obtained that IPs of iron clusters containing up to twenty atoms are determined by those of the central atoms (that is the IP of the cluster is coincided with that of Fe atom embedded in the centre of the jellium sphere with the radius of the cluster), and ones do not depend on the cluster geometry structure.

Our model calculations give the size dependence of IP which is in good qualitative agreement with the well-known experimental data (see Fig. 1). But our results predict the much larger amplitude of IP oscillations than the experiment. The oscillations on the calculated IP-curve are arisen from shell character of the model and the nonmonotonic occupation of the localized d-state of atoms of Fe clusters in dependence on the atom position in relation to the cluster surface as well as on the cluster size. (The occupation of localized d-states was chosen in accordance with the minimum of total energy of the system .)

Our calculations have shown that an IP of Fe microclusters consisting of up to 130 atoms does not reach the work function of bulk iron (4.5 - 4.8 eV). Apparently, the change from a Fe microclusters to solid state is occured for larger iron atomic aggregations.

3. REFERENCES

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