

First-Principles Study on Stability and Magnetism of MAI_n ($M = Ni, Cu$) ($n = 1 - 9$) Clusters

Baoxing Li*, Xiaojun Ren, Xiao Zhang, Zhiwei Ma, Jiaojiao Gu, Guobao Li

Department of Physics, Microfluidic Chip Institute, Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, Hangzhou Normal University, Hangzhou, China.

Email: *phybxli@yahoo.com.cn

Received April 28th, 2012; revised May 30th, 2012; accepted June 13th, 2012

ABSTRACT

We have investigated the structures, stabilities and magnetism of $NiAl_n$ and $CuAl_n$ ($n = 1 - 9$) clusters systematically by using first-principles density functional theory. Our calculated results indicate that most of the ground state structures for the Al clusters doped with one nickel or copper atom are different from those of the corresponding pure Al clusters. $NiAl_n$ and $CuAl_n$ ($n = 1 - 9$) cluster ions have similar geometrical configurations to the corresponding neutral clusters, except for positive $NiAl_9$ ion. The magnetic moments of $NiAl_n$ ($n = \text{odd number}$) and $CuAl_n$ ($n = \text{even number}$) cluster anions, neutrals and cations are 0, $1 \mu_B$, and $2 \mu_B$, respectively. The magnetic moments of $NiAl_4$ and $NiAl_6$ cluster anions, neutrals and cations are associated with $1 \mu_B$, $2 \mu_B$, and $3 \mu_B$, respectively. $NiAl_2$, $NiAl_8$ and $CuAl_n$ ($n = \text{odd number}$) clusters do not have any net magnetic moment. But, $NiAl_2$ and $NiAl_8$ cluster ions have the net magnetic moment of $1 \mu_B$.

Keywords: NiAl Cluster; CuAl Cluster; Stable Structure; Magnetism

1. Introduction

Transition-metal aluminides [1] and nickel-aluminum alloys [2] have attracted much attention due to their wide applications in advanced material technology. Both Al-based compounds of transition-metals (TM) [3] and nickel-based superalloys [4-6] are among the most promising candidates for high-performance structural materials. In the nanoscale regime, the nickel-aluminum bimetallic nanocluster has martensitic transformation as temperature alternation, which aroused many studies [7-10]. Their chemical and physical properties may vary with the composition, atomic ordering and the cluster size.

Wen *et al.* investigated Ni_nAl ($n = 2 - 8$) neutral clusters using the density functional theory based on generalized gradient approximation (GGA) with the exchange-correlation potential (BPW91) [7]. They found that atomization energies per atom for Ni_nAl ($n = 2 - 8$) clusters has the same trend as the binding energies per atom for Ni_n ($n = 3 - 9$) clusters. Ni_5Al is the relatively most stable structure in the series. Ni average magnetic moment decreases when alloyed with Al atoms than that in pure Ni clusters. Wang *et al.* [8] calculated the magnetic properties of MAI_n ($M = Cr, Mn, Fe, Co, Ni; n = 1 - 7, 12$)

clusters using density-functional theory based on generalized gradient approximation. They found that the MAI_n clusters have similar geometries as that of Al_{n+1} clusters. The computed total magnetic moments of the lowest-energy structures oscillate with the cluster size. Deshpande *et al.* reported the magnetic properties of small $Ni_{13-n}Al_n$ clusters with $n = 0 - 13$ calculated in the framework of density functional theory [9]. The overall magnetic moment of the $Ni_{13-n}Al_n$ cluster decreases as Al atoms increases. Bailey *et al.* presented their research results about nickel and aluminum clusters and nickel-aluminum nanoalloy clusters with up to 55 atoms. They investigated the effect of doping Al atoms into pure Ni clusters and *vice versa* [10].

In this paper, we will report our result about investigation on the $NiAl_n$ and $CuAl_n$ ($n = 1 - 9$) clusters by using first-principles calculations. Our calculations were performed with the generalized gradient approximation (GGA) by means of the Becke-Perdew functional, which uses Becke's [11] gradient correction to the local expression for the exchange energy and Perdew's [6] gradient correction to the local expression of the correlation energy, as implemented in the Amsterdam Density Functional (ADF) codes [12,13]. The self-consistent field was converged to a value of 10^{-6} .

Frequencies were computed using numerical different-

*Corresponding author.

tiation of gradients computed in slightly displaced geometries. The binding energy (BE) for the $NiAl_n$ cluster is calculated according to the following atomization reaction: $NiAl_n \rightarrow Ni + nAl$. It is defined by the following: $BE = E_{Ni} + nE_{Al} - E_{NiAl_n}$, where E is the total energy of the system. For the $CuAl_n$ cluster, similar calculation is made.

2. Results and Discussions

In order to reach the global minimum at energy surface, we chose a random way to produce initial geometrical configurations, and then used the Amsterdam Density Functional (ADF) package for geometrical optimizations. In this way, about one hundred thousand initial geometrical configurations are produced automatically within a three-dimensional box, or a cage, or a ball in real space. The separations of Al-Al, Ni-Al and Ni-Ni atoms are properly chosen to avoid overlapping or loosely packing. After the structural optimization on the initial configurations is performed, some of them are stable, but some structures are not convergent. In many cases, several different starting configurations are found to give the same structure upon optimization. A frequencies calculation has been performed to ensure that all the imaginary frequencies vanish and the structures are stable. Only the most stable structures for the Al_n ($n = 3 - 10$), $NiAl_n$, $CuAl_n$ ($n = 2 - 9$) clusters and their ions are presented in **Figures 1** and **2**. The similar structures for the cluster ions to their neutrals' are not plotted in the figures. But a different structure for $NiAl_9^+$ cluster from $NiAl_9$ cluster's is also presented in **Figure 1**.

$NiAl$ cluster is a dimer with different atoms. $NiAl_2$ cluster and its ions have an isosceles triangle with C_{2v} symmetry as their ground state structures. $NiAl_3$ cluster, its positive and negative ions have one three-dimensional tetrahedral structure with C_{3v} symmetry as their lowest energy structures, which are different from that of Al_4 cluster. Similarly, the ground state structure for $NiAl_4$, $NiAl_4^-$ and $NiAl_4^+$ clusters is one pentahedral structure with C_{4v} symmetry, differing from the planar structure of Al_5 cluster. The most stable structures for $NiAl_5$ cluster neutral, anion and cation have the same geometric configurations with C_s symmetry, which are obtained from the pentahedral structure of $NiAl_4$ by putting a surface Al atom. The lowest energy structures of $NiAl_6$ and $NiAl_8$ clusters cannot be obtained from Al_7 and Al_9 clusters by substituting one aluminum atom with nickel atom. Both of them have C_s symmetry. Al_7 cluster is an anti-trigonal prism with a capping atom (C_{3v} symmetry), while $NiAl_6$ cluster is a trigonal prism with a capping atom. The ground state structure for Al_9 cluster is regarded as a bi-capped hexagonal bipyramids with a capping atom. But $NiAl_8$ cluster possesses another different structure. For

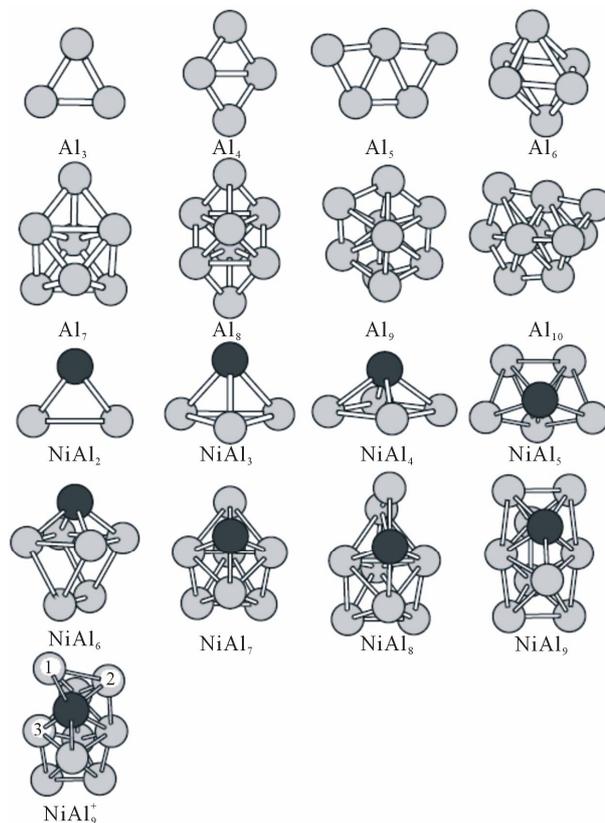


Figure 1. The ground state structures of Al_n ($n = 3 - 10$), $NiAl_n$ ($n = 2 - 9$) and $NiAl_n^+$ ion clusters. Larger black spheres and smaller gray sphere refer to Ni atom and Al atom, respectively.

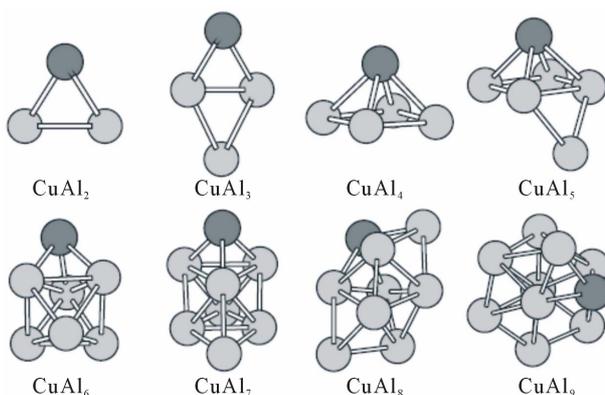


Figure 2. The ground state structures of $CuAl_n$ ($n = 2 - 9$) clusters. Larger black spheres and smaller gray sphere refer to Cu atom and Al atom, respectively.

$NiAl_7$ and $NiAl_9$ clusters, the lowest structures are different from those of pure Al_8 and Al_{10} clusters. It is worthy mentioning that positive $NiAl_9$ cluster ion has a severe distorted ground state structure compared with its neutral and anion (see $NiAl_9^+$ structure in **Figure 1**). Mulliken population analysis shows that the Al atoms labeled 1, 2 and 3 letters lose 37%, 28%, and 20% elec-

tron in the NiAl_9^+ structure, respectively. This makes the bond energies among them decrease. The severe structure distortion is mainly resulted from the non-uniform charge lose.

NiAl cluster has a single electron besides the paired electrons. If we add an electron into NiAl cluster, the electron would pair up with the original single electron, producing zero magnetic moment in NiAl^- cluster. But, the electron removed is from paired electrons in NiAl cluster. Thus, NiAl^+ cluster have two unpaired electrons, showing magnetic moment of $2 \mu_B$. Loss of an electron weakens the NiAl bond, which makes NiAl^+ cluster unstable due to positive binding energy. All the orbitals in neutral NiAl_2 cluster are doubly occupied. But the ionic clusters have the magnetic moment of $1 \mu_B$ because there is one single-occupied orbital. Interestingly, NiAl_4^- , NiAl_4 , and NiAl_4^+ clusters have magnetic moments of $1 \mu_B$, $2 \mu_B$ and $3 \mu_B$, respectively. It is found from observing **Table 1** that NiAl_3 , NiAl_5 , NiAl_7 , NiAl_9 clusters and their ions with odd-aluminum atoms have the same magnetic moments as NiAl cluster and their ions. That is to say, their anions have no magnetic moments, but the cations show the magnetic moment of $2 \mu_B$. NiAl_6^- , NiAl_6 , and NiAl_6^+ clusters have the same magnetic moments of $1 \mu_B$, $2 \mu_B$ and $3 \mu_B$ as NiAl_4^- , NiAl_4 , and NiAl_4^+ clusters, respectively. But, the magnetic properties of NiAl_8^- , NiAl_8 , and NiAl_8^+ clusters are the same as those of NiAl_2^- , NiAl_2 , and NiAl_2^+ clusters, respectively.

Figure 3 presents the calculated total density of states (DOS) for NiAl_4^- , NiAl_4 , NiAl_4^+ , and NiAl_6 clusters. DOS further provides an explanation of the magnetic behavior of these clusters. The majority spin is contributed by the Ni-d orbitals in the clusters. DOS for spin up

and spin down are asymmetric in the clusters suggesting the systems to be magnetic. Similar situations can be found in other clusters.

The magnetic moments of the Ni-Al clusters are considered to be from the strong sp-d hybridization. The electronic configurations of Ni atom and Al atom are $3d^8 4s^2$ and $3s^2 3p^1$, respectively. The Ni 3d orbitals are open shells. For the Ni-Al clusters, we note that the Ni atom obtain charge of about 0.4e from the Al atoms according to Mulliken populations. At the same time, some charge transfers into the 4p and 3d orbitals from the Ni 4s orbitals. For example, NiAl_3^+ cluster has magnetic moment of $2 \mu_B$, in which $0.494 \mu_B$ and $0.502 \mu_B$ are from the Ni atom and each Al atom, respectively. A part of the Ni 4s, Al 3s and 3p charge goes to the Ni 4p and 3d orbitals to form sp-d hybridization.

In order to better understand the role of the impurity Ni atom in the Al host clusters, we have also investigated the structural and magnetic properties of the copper-doped aluminum clusters by comparative study. The ground state structures for CuAl_n ($n = 2 - 9$) clusters are presented in **Figure 2**. Their magnetic moments, binding energies, energy gaps, electron affinities and ionization potentials are presented in **Table 2**. Although most of the structures can not be obtained from those of Al_n ($n = 3 - 10$) clusters either by replacing one Al atom with a Cu atom, more structures are similar to the lowest energy structures of Al_n ($n = 3 - 10$) clusters compared with NiAl_n ($n = 2 - 9$) clusters. It is found from observing the structures in **Figure 1** that some of the aluminum cluster structures get a cardinal change after doping one impurity nickel atom. But, one substitutional zinc atom only causes some local structural distortion without changing the basic geometrical configurations of the original Al_n

Table 1. The total magnetic moments (M , in μ_B) and the binding energies (BE , in eV) for NiAl_n ($n = 2 - 9$) clusters and their ions. The energy gaps (E_g , in eV), the electron affinities (EA , in eV) and ionization potentials (IP , in eV) of neutral NiAl_n ($n = 2 - 9$) clusters.

Clusters	M (in μ_B)			BE (in eV)			E_g (in eV)	EA (in eV)	IP (in eV)
	Anionic	Neutral	Cationic	Anionic	Neutral	Cationic			
NiAl	0	1	2	-4.82	-3.53	3.47	0.25	1.29	7.00
NiAl_2	1	0	1	-8.18	-6.94	-0.15	1.06	1.24	6.79
NiAl_3	0	1	2	-11.31	-9.92	-2.67	0.60	1.39	7.25
NiAl_4	1	2	3	-14.10	-12.21	-5.17	1.18	1.89	7.04
NiAl_5	0	1	2	-16.62	-14.59	-8.38	0.52	2.03	6.21
NiAl_6	1	2	3	-20.10	-17.64	-11.25	0.26	2.46	6.39
NiAl_7	0	1	2	-23.16	-21.06	-14.50	0.53	2.10	6.56
NiAl_8	1	0	1	-25.80	-23.56	-17.47	0.73	2.24	6.09
NiAl_9	0	1	2	-28.81	-26.39	-19.99	0.69	2.42	6.60

Table 2. The total magnetic moments (M , in μ_B) and the binding energies (BE, in eV) for $CuAl_n$ ($n = 2 - 9$) clusters and their ions. The energy gaps (E_g , in eV), the electron affinities (EA, in eV) and ionization potentials (IP, in eV) of neutral $CuAl_n$ ($n = 2 - 9$) clusters.

Clusters	M (in μ_B)			BE (in eV)			E_g (in eV)	EA (in eV)	IP (in eV)
	Anionic	Neutral	Cationic	Anionic	Neutral	Cationic			
CuAl	1	0	1	-3.58	-2.89	4.32	1.69	0.69	7.21
CuAl ₂	0	1	2	-6.23	-5.05	2.52	0.38	1.18	7.57
CuAl ₃	1	0	1	-8.91	-6.95	-0.73	0.36	1.96	6.22
CuAl ₄	0	1	2	-12.24	-10.06	-3.71	0.27	2.18	6.35
CuAl ₅	1	0	1	-14.67	-12.54	-6.18	0.65	2.13	6.36
CuAl ₆	0	1	2	-18.60	-15.95	-9.31	0.41	2.65	6.64
CuAl ₇	1	0	1	-20.92	-18.83	-12.75	0.90	2.09	6.08
CuAl ₈	0	1	2	-23.61	-21.32	-15.19	0.64	2.29	6.13
CuAl ₉	1	0	1	-26.88	-24.38	-18.15	0.68	2.50	6.23

($n = 3 - 10$) clusters [14]. This is considered to be related to the electronic configurations of the impurity atoms. As the number of electrons from Cr atom to Zn atom increases, the 3d orbital's hybridization intensity of metal atom with the orbital of Al reduces gradually. In addition, the cohesive energies of Ni, Cu, and Zn are 4.44, 3.49, and 1.35 eV, respectively [15]. Therefore, the influence of the impurity Cu atoms on the structures of the host Al clusters is less than that of the Ni atom. The influence caused by Zn atoms is even less.

Some of the ground state structures of $CuAl_n$ ($n = 2 - 9$) clusters are different from those of $NiAl_n$ ($n = 2 - 9$) clusters. They also present different magnetic properties. Note that the magnetic moments of all the anionic, neutral and cationic CuAl clusters with odd Al atoms are of 1 μ_B , 0, and 1 μ_B , respectively. But, the corresponding Cu-Al system containing even Al atoms are associated with the magnetic moments of 0, 1 μ_B , and 2 μ_B , respectively. The cations have two unpaired electrons, showing the magnetic moment of 2 μ_B .

Wang *et al.* [8] investigated the properties of MAI_n ($M = Cr, Mn, Fe, Co, Ni; n = 1 - 7, 12$) clusters. They found that the MAI_n clusters have similar structures to Al_{n+1} clusters. Our calculated ground state structures for Al_n ($n = 2 - 10$) clusters are in excellent agreement with the results reported in the Ref. [16], but differing from the structures obtained by Wang [8]. For $NiAl_n$ ($n = 5 - 7$) clusters, our structures are also different from Wang's. We performed further structural optimization calculations on their structures. As a result, the structures are unstable. Some of them transfer into our structures. The differences are probably caused by the different choice of the functional and the basis set for the problem under investigation. But, for the magnetic moments from NiAl

cluster to $NiAl_7$ cluster, our calculated results fully consistent with their results.

Figure 4 shows the second difference of cluster energies, $\Delta_2 E(n) = E(NiAl_{n-1}) + E(NiAl_{n+1}) - 2E(NiAl_n)$, which is a sensitive quantities that reflects the stabilities of clusters. The maxima can be found at $n = 2, 3, 7$ for $NiAl_n$ ($n = 1 - 9$) clusters, implying that the clusters are more stable than their neighboring clusters. But, for $CuAl_n$ ($n = 1 - 9$) clusters, the maxima can be found at $n = 2, 4, 6, 7$. Obviously, different impurity atoms would change their relative stabilities.

The electron affinities (EA) and ionization potentials (IP) of the mixed clusters as the function of the clusters size (shown as **Figure 4**) are also important quantities that reflect the stability of the clusters. The positive EAs imply that the clusters have a tendency to gain an electron under normal conditions. In the mixed $NiAl_n$ and $CuAl_n$ ($n = 1 - 9$) clusters, all the EAs are positive. Their trend is basically the same. The smaller clusters have a small electron affinity. However, for the ionization potentials, an opposite situation is observed. Generally speaking, the highly stable structure has small electron affinity and large ionization potential. For example, $NiAl_3$ and $NiAl_7$ clusters are comparatively highly stable. They have smaller EAs and larger IPs relative to their neighbors. **Figure 4** also presents the energy gaps (E_g) between the highest-occupied molecular orbital (HOMO) and the lowest-unoccupied molecular orbital (LUMO). Most of them are less than 1.0 eV.

3. Summary

We optimized the geometric structures of the mixed $NiAl_n$ and $CuAl_n$ ($n = 1 - 9$) clusters by using first-principles density functional theory. The ground state struc-

tures are obtained, and their relative stabilities are discussed. Most of the Al clusters doped one Ni or Cu atom are different from those of the host Al clusters. $NiAl_n$ and

$CuAl_n$ ($n = 1 - 9$) cluster ions present the similar structures to their neutral clusters. In addition, their magnetic properties are investigated. The magnetic moments of

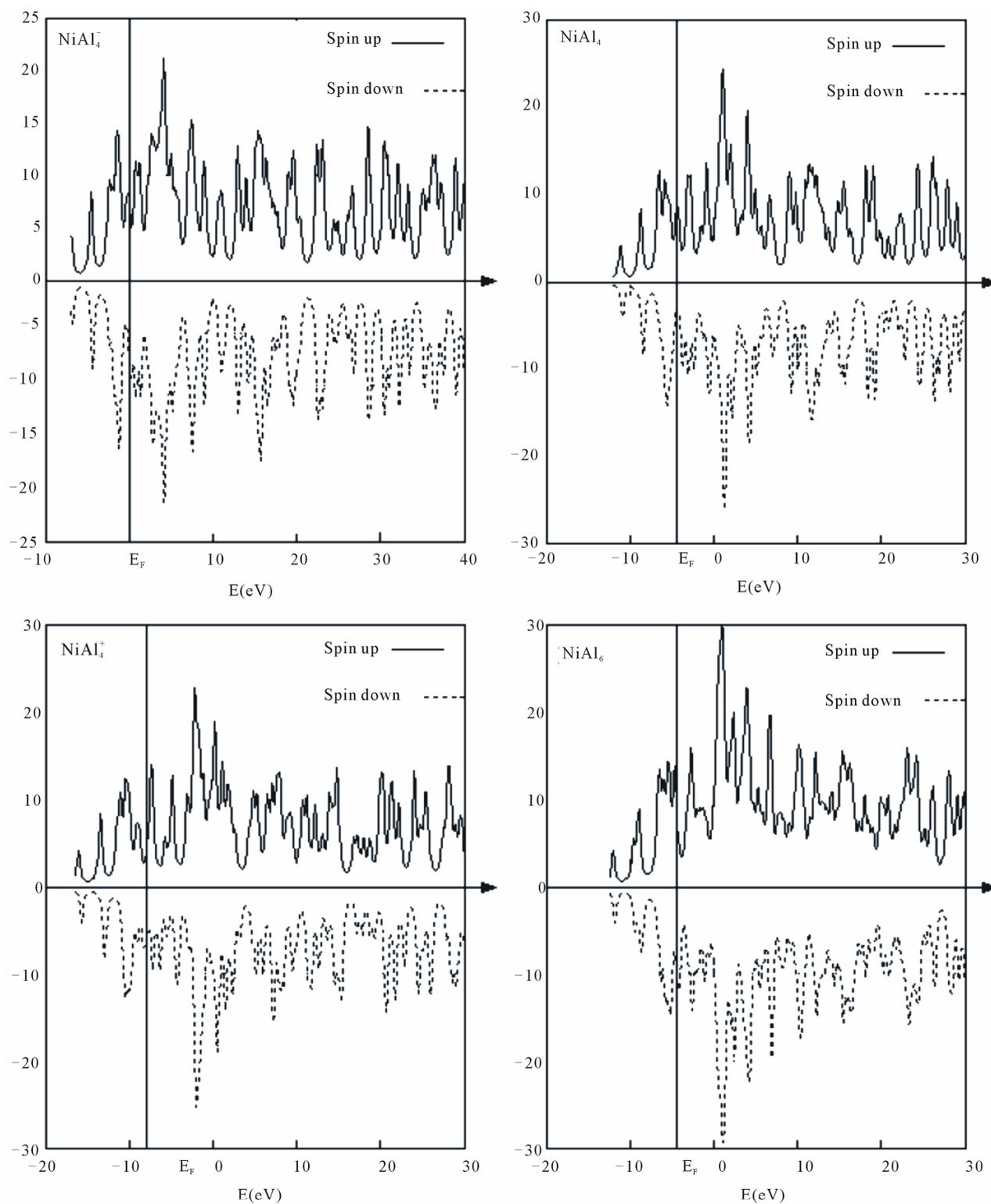


Figure 3. Total density of states (DOS) for $NiAl_4^-$, $NiAl_4$, $NiAl_4^+$, and $NiAl_6$ clusters. The Fermi level is given by a vertical line.

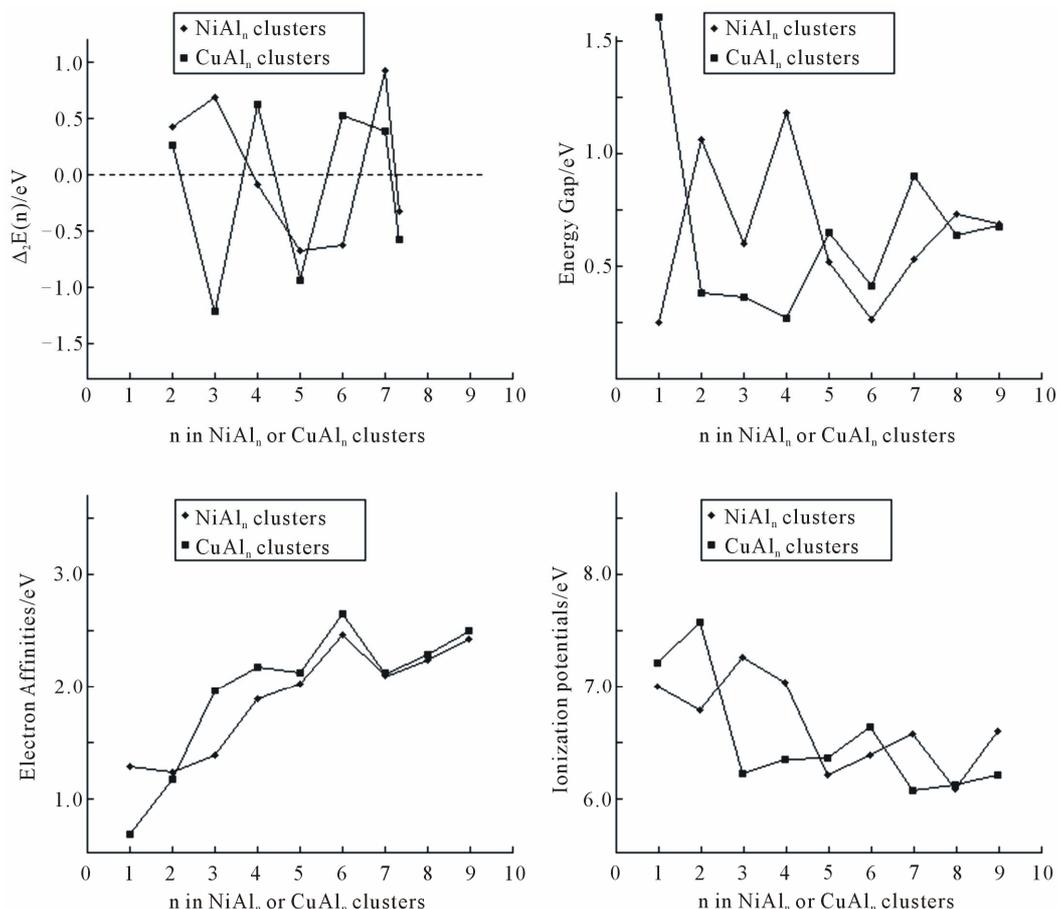


Figure 4. The second difference of cluster energies, the electron affinities, the ionization potentials, and the energy gaps E_g between the highest-occupied molecular orbital (HOMO) and the lowest-unoccupied molecular orbital (LUMO) of $NiAl_n$ and $CuAl_n$ ($n = 2 - 9$) clusters.

$NiAl_n$ ($n = \text{odd number}$) and $CuAl_n$ ($n = \text{even number}$) cluster anions, neutrals and cations are 0 , $1 \mu_B$, and $2 \mu_B$, respectively. Negative, neutral and positive $NiAl_4$ and $NiAl_6$ clusters show the magnetic moments of $1 \mu_B$, $2 \mu_B$, and $3 \mu_B$, respectively. $NiAl_2$, $NiAl_8$ and $CuAl_n$ ($n = \text{odd number}$) clusters do not have any magnetic moments, while $NiAl_2$ and $NiAl_8$ cluster ions have the magnetic moment of $1 \mu_B$. The magnetic moments of the Ni-Al clusters are from the strong sp-d hybridization.

4. Acknowledgements

A Foundation for the Author of National Excellent Doctoral Dissertation of PR China (Grant No. 200320), the Natural Science Foundation of Zhejiang Province (Grant No. Y6100098) supported this work.

REFERENCES

- [1] R. L. Fleischer, D. M. Dimidick and H. A. Lipsitt, "Intermetallic Compounds for Strong High-Temperature Materials: Status and Potential," *Annual Review of Materials Science*, Vol. 19, 1989, pp. 231-263.
- [2] A. N. Mansour, A. Dmitrienko and A. V. Soldatov, "Electronic Structure of Ni_3Al and $NiAl_3$ Alloys: mX-Ray-Absorption Fine-Structure Analysis," *Physical Review B*, Vol. 55, No. 23, 1997, pp. 15531-15536. [doi:10.1103/PhysRevB.55.15531](https://doi.org/10.1103/PhysRevB.55.15531)
- [3] B. Grushko and T. Ya. Velikanova, "Stable and Metastable Quasicrystals in Al-Based Alloy Systems with Transition Metals," *Journal of Alloys and Compounds*, Vol. 367, No. 1-2, 2004, pp. 58-63. [doi:10.1016/j.jallcom.2003.08.012](https://doi.org/10.1016/j.jallcom.2003.08.012)
- [4] H. S. Park, "Stress-Induced Martensitic Phase Transformation in Intermetallic Nickel Aluminum Nanowires," *Nano Letters*, Vol. 6, No. 5, 2006, pp. 958-962.
- [5] S. M. Shpiro, B. X. Yang, G. Shirane, Y. Noda and L. E. Tanner, "Neutron Scattering Study of the Martensitic Transformation in a Ni-Al β -Phase Alloy," *Physical Review Letters*, Vol. 62, No. 11, 1989, pp. 1298-1301. [doi:10.1103/PhysRevLett.62.1298](https://doi.org/10.1103/PhysRevLett.62.1298)
- [6] S. Rubini and P. Ballone, "Phonon Localization and Martensitic Transformation in Ni_xAl_{1-x} Alloys," *Physical Review B*, Vol. 50, No. 2, 1994, pp. 1297-1300. [doi:10.1103/PhysRevB.50.1297](https://doi.org/10.1103/PhysRevB.50.1297)

- [7] J. Q. Wen, Z. Y. Jiang, J. Q. Li, L. K. Cao and S. Y. Chu, "Geometrical Structures, Electronic States, and Stability of Ni_nAl Clusters," *International Journal of Quantum Chemistry*, Vol. 110, No. 7, pp. 1368-1375.
- [8] M. Wang, X. W. Huang, Z. L. Du and Y. C. Li, "Structural, Electronic, and Magnetic Properties of a Series of Aluminum Clusters Doped with Various Transition Metals," *Chemical Physics Letters*, Vol. 480, No. 4-6, 2009, pp. 258-264. [doi:10.1016/j.cplett.2009.09.027](https://doi.org/10.1016/j.cplett.2009.09.027)
- [9] M. D. Deshpande, R. Pandey, M. A. Blanco and A. Khalkar, "Magnetic Properties of $Ni_{13-n}Al_nNi_{13-n}Al_n$ Clusters with $n = 0 - 13$," *Journal of Nanoparticle Research*, Vol. 12, No. 4, 2010, pp. 1129-1136. [doi:10.1007/s11051-009-9654-6](https://doi.org/10.1007/s11051-009-9654-6)
- [10] M. S. Bailey, N. T. Wilson, C. Roberts and R. L. Johnston, "Structures, Stabilities and Ordering in Ni-Al Nanalloy Clusters," *The European Physical Journal D*, Vol. 25, No. 1, 2003, pp. 41-55. [doi:10.1140/epjd/e2003-00218-2](https://doi.org/10.1140/epjd/e2003-00218-2)
- [11] A. D. Becke, "Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior," *Physical Review A*, Vol. 38, No. 6, 1988, pp. 3098-3100. [doi:10.1103/PhysRevA.38.3098](https://doi.org/10.1103/PhysRevA.38.3098)
- [12] J. P. Perdew, "Density-Functional Approximation for the Correlation Energy of the Inhomogeneous Electron Gas," *Physical Review B*, Vol. 33, No. 12, 1986, pp. 8822-8824. [doi:10.1103/PhysRevB.33.8822](https://doi.org/10.1103/PhysRevB.33.8822)
- [13] ADF, "SCM, Theoretical Chemistry," Vrije Universiteit, Amsterdam, 2007. <http://www.scm.com>
- [14] X. J. Ren and B. X. Li, "First-Principles Study on Stability and Magnetism of Al_nZn ($n = 1 - 9$) Clusters," *Physica B*, Vol. 405, No. 9, 2010, pp. 2344-2349. [doi:10.1016/j.physb.2010.02.045](https://doi.org/10.1016/j.physb.2010.02.045)
- [15] P. H. T. Philipsen and E. J. Baerends, "Cohesive Energy of 3d Transition Metals: Density Functional Theory Atomic and Bulk Calculations," *Physical Review B*, Vol. 54, No. 8, 1996, pp. 5326-5333. [doi:10.1103/PhysRevB.54.5326](https://doi.org/10.1103/PhysRevB.54.5326)
- [16] F.-C. Chuang, C. Z. Wang and K. H. Ho, "Structure of Neutral Aluminum Clusters Al_n ($2 \leq n \leq 23$): Genetic Algorithm Tight-Binding Calculations," *Physical Review B*, Vol. 73, No. 12, 2006, pp. 1-7.