IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Study of the stable structures of the Ga_5As_5 cluster using the full-potential linear-muffin-tin-orbital molecular-dynamics method

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2002 J. Phys.: Condens. Matter 14 33

(http://iopscience.iop.org/0953-8984/14/1/304)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.238
The article was downloaded on 17/05/2010 at 04:42

Please note that terms and conditions apply.

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 33–43 PII: S0953-8984(02)26344-4

Study of the stable structures of the Ga_5As_5 cluster using the full-potential linear-muffin-tin-orbital molecular-dynamics method

Wei Zhao and Pei-lin Cao

Department of Physics and State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou, Zhejiang 310027, People's Republic of China

Received 27 June 2001, in final form 19 October 2001
Published 7 December 2001
Online at stacks.iop.org/JPhysCM/14/33

Abstract

We have investigated the structures and energies of a Ga_5As_5 cluster using full-potential linear-muffin-tin-orbital molecular-dynamics calculations. 27 stable structures were obtained for a Ga_5As_5 cluster, including all the structures considered by others. More importantly, we found a new ground state, a two-capped cube, the energy of which is lower than that of the others. Furthermore, we found that the two-capped cube structure presented semiconductor-like properties through the calculation of the density of states.

1. Introduction

It is obvious that the study of clusters is important for understanding the nature of transitional forms between atoms and bulk. Recently, the structure of small clusters has been a subject of great interest in both experimental and theoretical studies [1, 2]. Among the mixed clusters, GaAs clusters have been the focus of particularly many investigations due to their importance in constructing fast microelectronic devices [3]. Experimentally, laser vaporization followed by supersonic expansion was used to produce clusters of GaAs and their positive and negative ions [4–6]. On the other hand, theoretical studies of larger mixed clusters have been comparatively limited due to the computational difficulties associated with the structural as well as permutational variations resulting from the presence of more than one element. Only a few studies of small GaAs clusters have been reported, recently [7–11].

Recently, we used full-potential linear-muffin-tin-orbital molecular-dynamics (FP-LMTO MD) calculations to study the structures and energies of the small clusters Ga_4As_4, Ge_n and Si_n (n up to 60) [12–17]. This method was verified as being an accurate method for studying the semiconductor cluster structures. Because some different ground-state structures were suggested by others for a Ga_5As_5 cluster, we find it even more important to go on to study the structures and energies of a Ga_5As_5 cluster using the FP-LMTO MD method. For a Ga_5As_5 cluster, Lou *et al* [7] came up with two structures using the Dmol method whose energies were comparatively low, a tetracapped trigonal prism (TTP) structure which is considered as

 © 2002 IOP Publishing Ltd Printed in the UK

the lowest-energy structure and a tetracapped octahedral structure. Andreoni [8] considered three structures using the cp method. Vasiliev *et al* [10] studied the absorption spectra of two Ga_5As_5 clusters using a time-dependent density-functional formalism within the local density approximation. Yi [11] considered one structure using the cp method, a cube-based structure, which is considered as the most stable structure.

In this paper, we present 27 stable structures of a Ga_5As_5 cluster. The ground-state structure that we obtained is a two-capped cube structure.

2. Method

The FP-LMTO method [18–21] is a self-consistent implementation of the Kohn–Sham equations in the local density approximation [22]. In this method, space is divided into two parts: non-overlapping muffin-tin (MT) spheres centred at the nuclei and the remaining interstitial region. LMTOs are augmented Hankel functions, and are augmented inside the MT spheres, but not in the interstitial region [23–25]. In LMTO method, one thing that we must do is to calculate the interstitial-potential matrix elements:

$$V_{ij}^{I} = \int_{I} \phi_i(x) V_I(x) \phi_j(x)\,\mathrm{d}x \tag{1}$$

where I is the interstitial region, V_I is the interstitial potential, i and j are abbreviations for νL and $\nu' L'$, respectively, ϕ_i is a LMTO envelope function centred at site ν with angular momentum L and L is an abbreviation for the angular-momentum quantum numbers (l, m). In different methods, we handle V_{ij}^{I} in different ways. In the FP-LMTO method for clusters, Methfessel *et al* [20, 21] used non-overlapping MT spheres. They retained non-spherical potential terms inside the MT spheres, but expanded the interstitial potential $V_I(x)$ in a different set of atom-centred Hankel functions. In order to obtain the interstitial-potential matrix elements, we need an accurate representation, valid in the interstitial region, of the product of two Hankel functions centred at the same or at different sites. That is, we require an expansion of the form

$$\phi_i^* \phi_j = \sum_k C_k^{ij} \chi_k(x) \tag{2}$$

where i and j are abbreviations for νL and $\nu' L'$, respectively, ϕ_i is a LMTO envelope function centred at site ν with angular momentum L, L is an abbreviation for the angular-momentum quantum numbers (l, m), k is an abbreviation for $(\nu L \alpha)$, the index α runs over different locations, χ_k are functions of the charge density Hankel function set and C_k^{ij} are expansion coefficients. The interstitial-potential matrix element V_{ij}^{I} then reduces to a linear combination of integrals of the functions χ_k times the interstitial potential. Because the interstitial potential itself is also expanded in functions of the χ_k type, the desired interstitial integral has now been expressed as a linear combination of integrals of products of pairs of Hankel functions; i.e., the three-centre integral has been reduced to a sum of two-centre integrals. Because the products are smooth functions, the coefficients in equation (2) above can be adjusted until the best fit of the values and slopes of the right-hand side to the values and slopes of the products is obtained for all spheres simultaneously by a tabulation technique applied to the surfaces of the spheres. In the cluster method, the expansion is first calculated for two atoms arranged along the z-axis and the coefficients are tabulated as functions of the interatomic distance. For general geometry, the expansion is obtained by rotating the tabulated fit using the rotation matrices of the spherical harmonics. The tabulated fit is obtained by direct numerical integration and can be made as accurate as desired [19]. The force expression for the FP-LMTO method can be obtained using the Harris energy function [18, 19]. During the optimization of one structure, no restriction is imposed. Starting with one geometric configuration, we set up one time step.

Table 1. The relative energy (eV) for the structures of the Ga_5As_5 cluster with respect to that of the most stable structure a1, which was set to 0 eV. (The total energy of a1 is −564 684.756 eV.)

Structure	a1	a2	a3	a4
Energy	0.000	1.282	2.598	2.719
Structure	a5	a6	b1	b2
Energy	2.880	3.894	1.752	1.944
Structure	b3	c1	c2	c3
Energy	2.454	0.193	0.485	0.936
Structure	c4	c5	c6	c7
Energy	0.947	1.683	2.181	2.874
Structure	c8	c9	d1	d2
Energy	3.771	6.160	1.750	1.752
Structure	d3	d4	d5	d6
Energy	1.861	2.422	0.717	3.059
Structure	d7	e1	e2	
Energy	3.445	3.033	3.135	

In each time step, the eigenvalue problem is solved exactly and the output density is admixed with the input density in the usual way. The nuclei are then moved according to the forces using the Verlet algorithm. We then decompose the mixed density, move each partial density along with its atom and re-overlap at the new geometry. After many iterations, the maximum of the forces is less than 0.001 au, and the total energy stays nicely constant because the system stays close to self-consistency (so the nearly zero forces agree with the energy minima). The process is stopped when the self-consistency condition is met.

3. Results and discussion

The permutational possibilities of arranging ten atoms to form a mixed cluster are numerous. In order to systematize the search for the equilibrium structure of the Ga_5As_5 cluster, possible initial configurations must be defined as seeds. Because of the similarities between Ga_5As_5 and Ge_{10} clusters, the search began by defining possible geometries using the geometries previously optimized for Ge_{10} [17] and Ga_5As_5 clusters considered by others [7–11].

The 27 stable structures of the Ga_5As_5 cluster that we obtained are shown in figure 1. Their energies are shown in table 1, and the coordinates of the 14 stable structures, the energies of which are lower than those of the others, are shown in table 2. Their energy diagram is shown in figure 2.

The equilibrium structures of the Ga_5As_5 cluster that we obtained can be classified into five groups according to structural resemblance: the two-capped cube structure (a1–a6), the two-capped antitetragonal prism (b1–b3), the four-capped octahedrons (c1–c9), the four-capped trigonal prisms (d1–d7) and the three-capped pentagonal bipyramids (e1–e2).

The first structures of the Ga_5As_5 cluster are the two-capped cube structures (a1–a6). a1 is a minimum-energy structure, which is the most stable among these 27 stable structures. a2 is considered by Andreoni [8] and found to be 1.282 eV less stable than a1. The structure a3 is considered as the most stable by Yi [11], but we find that the energy of a3 is 1.598 eV less stable than a1. a4 and a5 are found to be 2.719 eV and 2.880 eV less stable than a1, respectively. a6 is the least stable among the six structures, and it is found to be 3.894 eV less stable than a1.

The second structures are the two-capped antitetragonal prisms (b1–b3) and we also considered the two-capped severely distorted cube structure. b1 is the most stable among

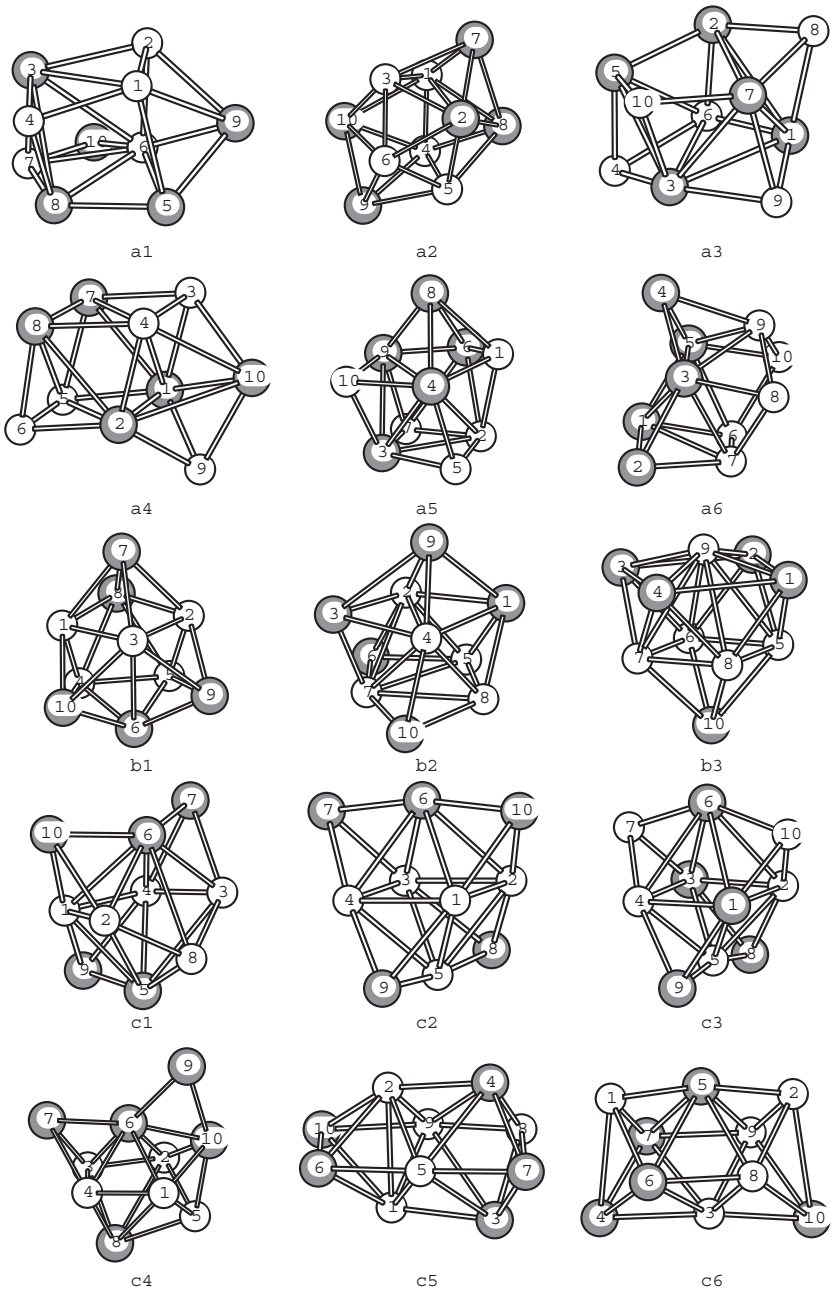

Figure 1. Geometries of 27 stable structures of the Ga_5As_5 cluster. The grey (white) circles are the Ga (As) atoms.

the three structures and found to be 1.752 eV less stable than a1. b2 and b3 are found to be 0.192 and 0.702 eV less stable than b1. Moreover, from our molecular-dynamics calculations we find that the two-capped cube structure is easy to form for a Ga_5As_5 cluster, because several different types of initial structure all transform to the two-capped cube structure.

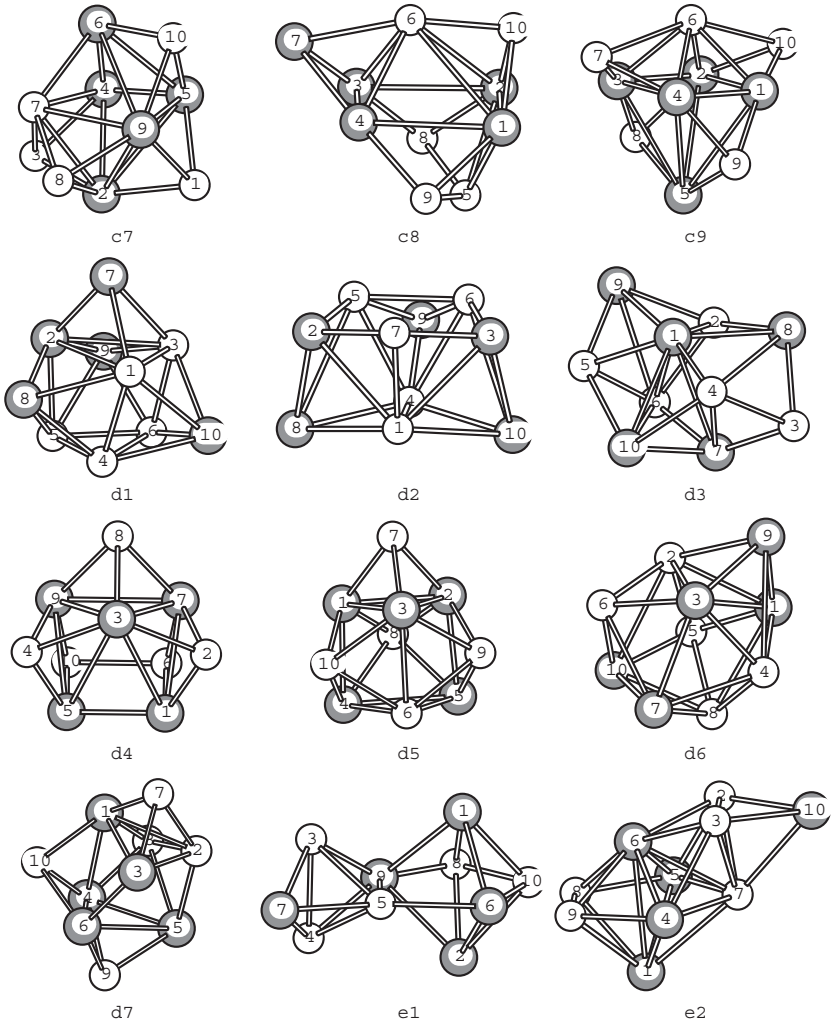

Figure 1. (Continued)

The third structures are the four-capped octahedrons (c1–c9). c1 is the most stable among the nine structures and found to be only 0.193 eV less stable than a1. c1, the TO structure, was also considered by Lou *et al* [7] and they found a couple of different atomic arrangements with similar energies for this type of structure. From our calculations, we also find structures of this type—such as c2 and c3—whose energy is comparatively low among those of the 27 structures. c2 and c3 are found to be 0.292 and 0.743 eV less stable than c1. c3 was also considered by Andreoni [8]. c4 and c5 are found to be 0.754 and 1.490 eV less stable than c1. Structure c6 is formed by a three-capped pentagonal bipyramid undergoing further distortion and found to be 1.988 eV less stable than c1. c7 and c8 are found to be 2.681 and 3.578 eV less stable than c1. Structure c9 is the least stable among the 27 structures and found to be 6.160 eV less stable than a1.

The fourth structures are the four-capped trigonal prisms (d1–d7). d1 is the most stable among the seven structures and was also considered by Lou *et al* [7] (as a TTP structure) and by Andreoni [8]. d2 and d4 are found to be 0.002 and 0.672 eV less stable than d1. Structure d3 is

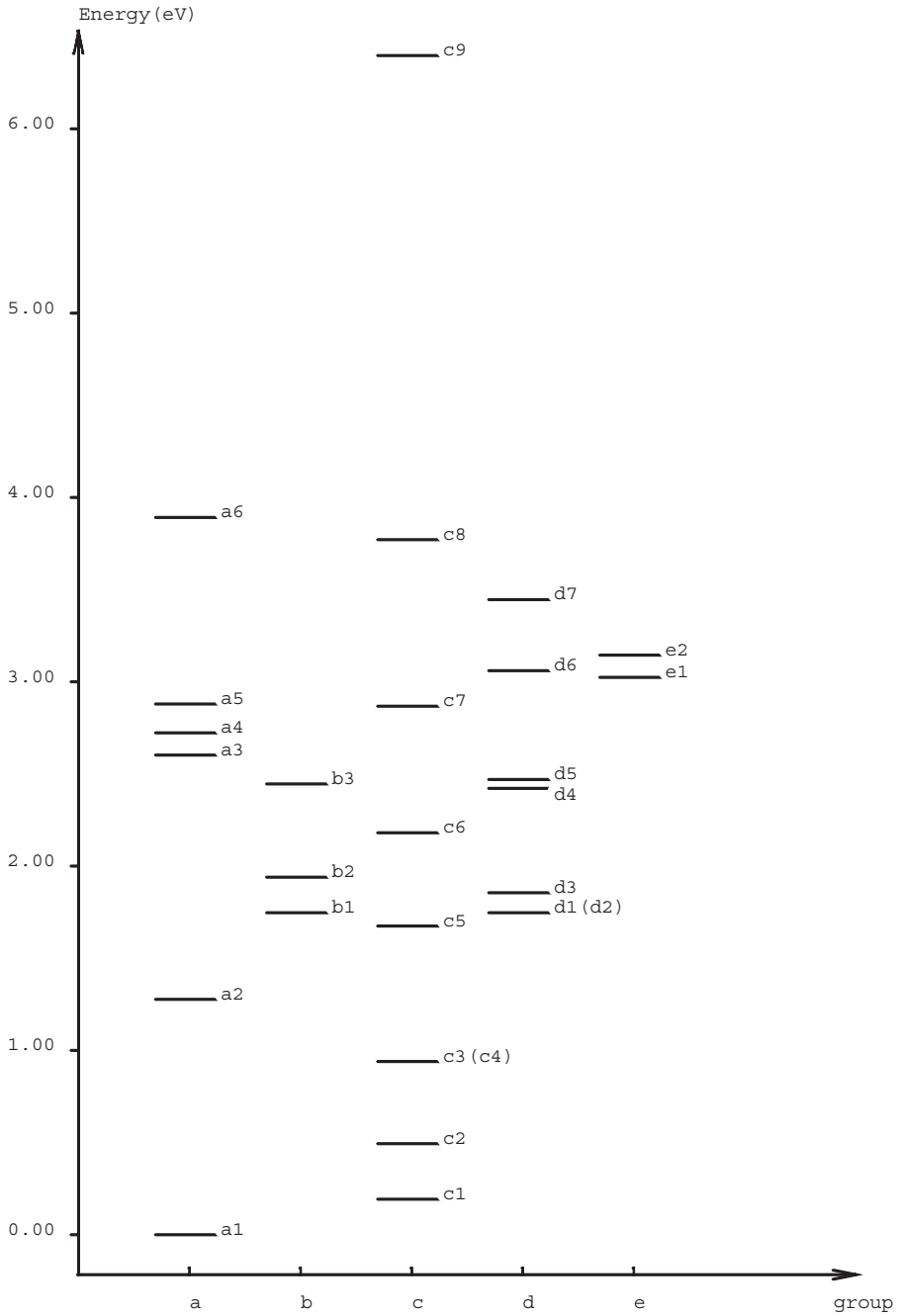

Figure 2. The energy diagram of the Ga_5As_5 cluster; the y-axis represents the relative energy (eV) with respect to that of the lowest-energy structure and the x-axis represents a catalogue of G_5A_5 clusters.

formed by a three-capped pentagonal bipyramid undergoing further distortion and found to be 0.111 eV less stable than d1. d5 and d6 are found to be 0.717 and 1.309 eV less stable than d1. d7 is the least stable among the seven structures and found to be 1.695 eV less stable than d1.

Table 2. The coordinates for the fourteen structures which were the most stable ones among the 27 structures of the G_5A_5 cluster.

Structure	Atom type	x (au)	y (au)	z (au)
a1	1(As)	1.987 13	−2.254 74	3.400 11
	2(As)	2.539 13	2.464 80	3.124 72
	3(Ga)	−2.379 86	1.899 53	2.334 09
	4(As)	−2.585 05	−2.827 83	2.237 46
	5(Ga)	3.046 70	−2.902 28	−1.934 90
	6(As)	2.205 95	2.611 59	−1.758 33
	7(As)	−2.623 38	2.811 15	−2.399 83
	8(Ga)	−1.619 71	−1.782 57	−2.199 04
	9(Ga)	6.090 44	−0.084 87	0.498 54
	10(Ga)	0.211 49	6.842 47	−3.459 82
a2	1(As)	−3.236 03	−0.474 05	−0.216 04
	2(Ga)	2.211 31	1.737 75	−0.553 40
	3(As)	0.803 59	−3.115 36	−0.134 36
	4(As)	−3.644 51	1.030 92	−4.765 01
	5(As)	0.811 95	2.573 92	−5.316 73
	6(As)	2.938 84	−1.711 72	−4.291 53
	7(Ga)	−0.266 96	1.132 96	3.604 58
	8(Ga)	−2.079 46	4.638 49	−1.372 86
	9(Ga)	−0.605 58	−1.625 18	−8.297 69
	10(Ga)	−1.855 67	−4.263 95	−4.119 40
b1	1(As)	−3.340 38	−1.007 37	−0.456 00
	2(As)	2.542 59	2.388 23	−0.453 71
	3(As)	1.315 57	−2.280 45	0.426 18
	4(As)	−3.081 99	0.503 12	−4.937 31
	5(As)	1.108 44	2.920 61	−4.935 79
	6(Ga)	1.185 24	−2.053 04	−5.294 95
	7(Ga)	−0.970 05	1.677 40	3.200 01
	8(Ga)	−2.439 52	4.226 33	−1.300 35
	9(Ga)	5.255 39	−1.213 36	−2.763 39
	10(Ga)	−1.576 96	−5.158 64	−2.763 79
b2	1(Ga)	−2.033 25	4.394 48	−0.333 01
	2(As)	−2.399 01	−0.686 27	−2.214 65
	3(Ga)	−1.497 06	−4.414 05	1.190 55
	4(As)	−0.412 79	0.328 45	2.871 68
	5(As)	1.085 18	2.411 71	−3.794 09
	6(Ga)	1.087 77	−2.434 20	−5.279 64
	7(As)	2.594 42	−2.655 88	−0.721 04
	8(As)	2.805 92	3.284 31	0.585 34
	9(Ga)	−5.225 18	0.461 78	1.695 65
	10(Ga)	4.422 01	−0.695 29	3.267 34
c1	1(As)	2.470 76	−2.392 28	−0.188 87
	2(As)	3.577 00	2.380 88	−0.129 27
	3(As)	−3.576 61	2.381 44	−0.127 78
	4(As)	−2.472 91	−2.391 64	−0.190 66
	5(Ga)	0.000 92	−0.117 55	−4.486 71
	6(Ga)	0.000 38	1.655 68	3.347 07
	7(Ga)	−4.297 29	−0.405 64	4.090 18
	8(As)	−0.000 61	4.200 89	−2.583 73

Table 2. (Continued)

Structure	Atom type	x (au)	y (au)	z (au)
	9(Ga)	0.000 37	−4.868 97	−3.827 02
	10(Ga)	4.298 17	−0.404 92	4.089 73
c2	1(As)	2.710 27	−2.521 09	−0.032 17
	2(As)	2.710 27	2.521 09	−0.032 17
	3(As)	−2.710 24	2.520 97	−0.031 83
	4(As)	−2.710 24	−2.520 97	−0.031 83
	5(As)	−0.000 21	0.000 00	−3.807 34
	6(Ga)	0.000 33	0.000 01	4.007 74
	7(Ga)	−4.885 60	−0.000 01	3.521 70
	8(Ga)	−0.000 43	4.885 50	−3.554 25
	9(Ga)	−0.000 43	−4.885 50	−3.554 25
	10(Ga)	4.886 30	0.000 00	3.521 30
c3	1(Ga)	2.664 62	−3.303 96	0.070 59
	2(As)	2.547 78	2.839 55	0.022 24
	3(Ga)	−2.661 92	3.305 36	0.070 84
	4(As)	−2.545 80	−2.839 01	0.024 26
	5(As)	0.000 12	−0.000 20	−3.279 00
	6(Ga)	−0.002 29	−0.005 87	4.495 37
	7(As)	−4.317 05	0.131 91	3.106 06
	8(Ga)	−0.344 66	4.920 46	−3.816 55
	9(Ga)	0.345 30	−4.920 64	−3.816 61
	10(As)	4.313 98	−0.127 93	3.108 26
c4	1(As)	0.829 73	−3.452 12	−1.489 61
	2(As)	0.829 52	3.452 23	−1.489 78
	3(As)	−3.463 61	2.447 62	0.491 66
	4(As)	−3.463 51	−2.447 67	0.491 71
	5(As)	1.240 83	−0.000 01	−4.757 24
	6(Ga)	0.538 11	0.000 14	2.521 37
	7(Ga)	−3.770 30	0.000 02	5.127 89
	8(Ga)	−3.947 63	−0.000 11	−3.936 26
	9(Ga)	5.480 48	−0.000 31	4.064 68
	10(Ga)	4.392 77	0.000 21	−0.799 65
c5	1(As)	−2.670 31	−3.081 89	0.133 01
	2(As)	−2.670 31	3.081 90	0.133 01
	3(Ga)	2.387 19	−3.537 47	−0.234 90
	4(Ga)	2.387 19	3.537 47	−0.234 90
	5(As)	−0.320 06	0.000 00	3.132 89
	6(Ga)	−5.326 32	0.000 00	3.628 30
	7(Ga)	4.751 32	0.000 00	2.334 34
	8(As)	2.955 90	0.000 00	−3.544 25
	9(As)	−1.711 57	0.000 00	−3.479 75
	10(Ga)	−6.618 39	0.000 00	−1.811 52
c6	1(As)	−3.683 77	0.705 24	−0.000 31
	2(As)	4.209 84	4.687 38	0.000 05
	3(As)	3.170 06	−2.585 47	0.000 18
	4(Ga)	−1.527 82	−5.033 60	−0.000 01
	5(Ga)	0.004 89	3.154 83	−0.000 17
	6(Ga)	−0.743 13	−1.333 56	3.385 37
	7(Ga)	−0.742 74	−1.333 79	−3.385 54

Table 2. (Continued)

Structure	Atom type	x (au)	y (au)	z (au)
	8(As)	3.734 83	1.042 40	3.264 97
	9(As)	3.735 19	1.042 26	−3.264 73
	10(Ga)	7.794 98	−0.710 68	0.000 19
d1	1(As)	−3.124 85	−0.456 66	−0.066 68
	2(Ga)	1.723 21	2.984 06	−0.433 57
	3(As)	1.166 70	−2.934 21	−0.066 21
	4(As)	−3.060 11	0.318 20	−4.806 69
	5(As)	1.333 42	2.310 00	−5.257 61
	6(As)	1.805 79	−2.490 82	−4.806 43
	7(Ga)	0.383 93	0.665 54	3.450 26
	8(Ga)	−2.681 19	4.427 37	−2.082 27
	9(Ga)	5.174 74	−0.108 54	−2.082 35
	10(Ga)	−2.700 35	−4.678 27	−3.157 22
d2	1(As)	−3.095 94	0.000 05	0.394 10
	2(Ga)	0.822 01	3.725 57	−0.180 42
	3(Ga)	0.822 25	−3.725 32	−0.180 54
	4(As)	−2.391 06	−0.000 51	−4.571 44
	5(As)	1.940 64	2.393 60	−4.723 19
	6(As)	1.940 63	−2.393 80	−4.723 50
	7(As)	1.091 25	0.000 07	2.602 62
	8(Ga)	−3.455 08	4.553 91	−2.461 22
	9(Ga)	0.663 10	0.000 75	−9.158 09
	10(Ga)	−3.455 10	−4.554 27	−2.460 40
d3	1(Ga)	0.163 56	0.994 36	2.194 42
	2(As)	3.957 67	−1.200 47	0.472 49
	3(As)	−3.529 41	−4.128 11	−1.516 64
	4(As)	−4.175 33	−0.348 56	1.385 41
	5(As)	0.952 55	5.402 46	0.829 60
	6(As)	2.383 23	2.151 72	−2.552 40
	7(Ga)	−1.873 30	−0.303 66	−3.306 71
	8(Ga)	0.022 16	−4.487 12	1.751 66
	9(Ga)	5.371 54	3.192 53	2.446 74
	10(Ga)	−3.241 99	3.994 26	−1.601 50
d4	1(Ga)	2.372 20	−2.743 97	2.076 51
	2(As)	4.325 70	1.504 12	2.666 76
	3(Ga)	0.000 11	3.065 25	1.956 84
	4(As)	−4.327 30	1.506 53	2.667 77
	5(Ga)	−2.374 55	−2.740 40	2.077 05
	6(As)	2.397 88	−3.574 03	−2.594 83
	7(Ga)	3.039 88	1.023 20	−1.861 66
	8(As)	0.001 30	4.479 20	−2.540 81
	9(Ga)	−3.039 39	1.025 72	−1.861 15
	10(As)	−2.394 03	−3.571 32	−2.593 10

The final structures are the three-capped pentagonal bipyramids (e1–e2). Their energies are comparatively high among those of the 27 stable structures: 3.033 and 3.135 eV less stable than a1, respectively. This is different from the case for a Ga_4As_4 cluster, whose ground-state structure is a capped pentagonal bipyramid.

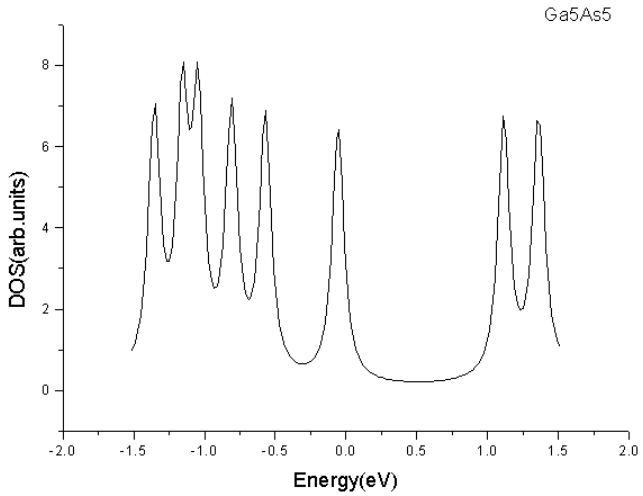

Figure 3. The electronic density of states for the a1 structure in figure 1. The density of states shows a gap of 1.17 eV.

These stable structures that we obtained include all the structures considered by others. Furthermore, we obtained another ground-state structure: a two-capped cube structure (a1). As regards structure d1, the TTP structure considered as the most stable structure by Lou *et al* [7], we find that its energy is 1.750 eV less stable than a1. We find that the energy of structure c1, the TO structure considered by Lou *et al* [7], is very low—only 0.193 eV less stable than a1. According to [8], structures a2 and d1 are quasidegenerate and structure c3 is found to be 1.2 eV less stable than a2 and d1. But we find that a2 is 0.468 eV more stable than d1 and that c3 is 0.346 eV more stable than a2. a3 was considered as the most stable structure by Yi [11], but we find that structure a3 is 2.598 eV less stable than a1. Moreover, we also find that structure d5 is analogous to the Ga_5As_5 cluster proposed by Vasiliev *et al* [10], but we find that d5 is 0.717 eV less stable than d1.

Furthermore, we also calculated the density of states of the structure a1. Figure 3 shows the calculated density of electronic states, where the DOS is plotted as a function of the energy. The density of states shows a gap of 1.17 eV, presenting semiconductor-like properties. In plotting the DOS for the structure a1, each discrete energy level is broadened by a Gaussian with full width at half-maximum (FWHM) given by 0.05 eV.

4. Conclusions

Using the FP-LMTO MD method, we performed calculations on the structures and energies of the Ga_5As_5 cluster. We obtained 27 stable structures of the cluster. Among these, the two-capped cube structure (a1) is the most stable structure and the four-capped octahedron (c9) is the least stable. Through the calculation of the density of states of the a1 structure, we found that it presented semiconductor-like properties.

Acknowledgment

This project was supported by the National Natural Science Foundation of China, No 19874052.

References

[1] Jena P, Khanna S N and Rao B K (ed) 1992 *Physics and Chemistry of Finite Systems: From Clusters to Crystals* (Deventer: Kluwer)
[2] Bernstein E R 1989 *Atomic and Molecular Clusters (Studies in Physical and Theoretical Chemistry 68)* (Amsterdam: Elsevier)
[3] Howes M J and Morgan D V (ed) 1985 *Gallium Arsenide: Materials, Devices, and Circuits* (New York: Wiley)
[4] O'Brien S C, Liu Y, Zhang Q, Heath J R, Tittle F K, Curl R F and Smalley R E 1986 *J. Chem. Phys.* **84** 4074
[5] Liu Y, Zhang Q-L, Tittle F K, Curl R F and Smalley R E 1986 *J. Chem. Phys.* **85** 7434
[6] Zhang Q-L, Liu Y, Curl R F, Tittle F K and Smalley R E 1988 *J. Chem. Phys.* **88** 1670
[7] Lou L, Wang L, Chibante L P F, Laaksonen R T, Nordlander P and Smalley R E 1991 *J. Chem. Phys.* **94** 8015
[8] Andreoni W 1992 *Phys. Rev.* B **45** 4203
[9] Lou L, Nordlander P and Smalley R E 1992 *J. Chem. Phys.* **97** 1858
[10] Vasiliev L, Ogut S and Chelikowsky J R 1999 *Phys. Rev.* B **60** 8477
[11] Yi Jae-Yel 2000 *Chem. Phys. Lett.* **325** 269
[12] Zhao Wei, Cao Pei-lin, Li Bao-xing, Song Bin and Nakamatsu H 2000 *Phys. Rev.* B **62** 17 138
[13] Li B X, Qiu M and Cao P L 1999 *Phys. Lett.* A **256** 386
[14] Li B X, Jiang M and Cao P L 1999 *J. Phys.: Condens. Matter* **11** 8517
[15] Qiu Min, Jiang Ming, Zhao Yu-Jun and Cao Pei-lin 1999 *J. Chem. Phys.* **110** 10 738
[16] Li B X, Que D L and Cao P L 2000 *Phys. Rev.* B **61** 1685
[17] Li B X and Cao P L 2000 *Phys. Rev.* B **62** 15 788
[18] Methfessel M and Schilfgaarde M V 1993 *Int. J. Mod. Phys.* B **7** 262
[19] Methfessel M and Schilfgaarde M V 1993 *Phys. Rev.* B **48** 4937
[20] Methfessel M 1988 *Phys. Rev.* B **38** 1537
[21] Methfessel M, Rodriguez C O and Andersen O K 1989 *Phys. Rev.* B **40** 2009
[22] Kohn W and Sham L J 1965 *Phys. Rev.* **140** A1133
[23] Andersen O K 1975 *Phys. Rev.* B **12** 3060
[24] Andersen O K and Woolley R G 1975 *Mol. Phys.* **26** 905
[25] Springborg M and Andersen O K 1975 *J. Chem. Phys.* **87** 7125