Si M

Si_n

$n = 2, 3, 4$

D_0

1967
102

Goldfinger P.

La chimica e l'industria, 49, N1, 51

Химическая и физическая устойчивость простых газообразных молекул.

☒

Массспектр.

1972

Si_n^{2+}

9267k **Divalent polyatomic ions in the mass spectra of silicon by high-frequency sparks.** Vidal, Georges (Off. Natl. Etud. Rech. Aerosp., Chatillon-sous-Bagneux, Fr.). *Int. J. Mass Spectrom. Ion Phys.* 1972, 10(2), 204–6 (Fr). Mass spectra of highly pure Si samples showed 4 unexpected lines at at. masses of 42.5, 56.5, 57.5, and 84.5. They correspond to $^{28+28+29}Si_3^{2+}$, $^{28+28+28+29}Si_4^{2+}$, $^{28+28+29+30}Si_4^{2+}$, and $^{28+28+28+28+28+29}Si_6^{2+}$, resp.

C.A. 1973, <u>78</u> № 2.

Si_5

Anderson Alfred B.

1975

„J. Chem Phys" 1975,

<u>63</u>, N 10, 4430-36 (англ)

(см C_2; <u>III</u>)

парам.
решетки
сил. пост.
эн. связи

*4-10911

50606.430
Ph,MGU,TC

Si_n^- 76237 (Ae) стаб. гидрид.

1975
*4-8980

Leleyter M., M^{lle}, Joyes P. Etude expérimentale et théorique de l'émission secondaire d'ions molécualaires. [illegible] cas des éléments du groupe IV-B. "J. phys." (France), 1975, 36, № 5, 343-355
(франц., рез. англ.) 0301 пик

361 361 373 ВИНИТИ

Si_n (кластеры)

1981

$n = 13, 16, 19$

расчет

14 Б22. Расчет электронного строения вакансий и хемисорбционной связи на поверхности Si(111) кластерным методом X_α-дискретного варьирования. Tsukada Masaru, Hoshino Toshiharu. Electronic structure of vacancy and chemisorptive bond on Si(111) surface by the DV—X_α cluster calculation. «Int. J. Quantum. Chem.», 1981, Quantum. Chem. Symp. № 15, 445—455 (англ.)

Методом X_α-дискретного варьирования проведены расчеты кластеров, моделирующие (111)-поверхность кремния, содержащие 13, 16 и 19 атомов Si. Границы кластера насыщались атомами водорода. Показано, что кластер Si_{13} воспроизводит основные характеристики фотоэлектронных спектров (111)-поверхности кремния. Обсуждено электронное строение вакансий и влияние искажения геометрии кластеров на плотность состояний. Показано, что поверхн. вакансии необходимы для того, чтобы получить электронное строение, хорошо со-

Х. 1982, 19, N 14.

гласующееся с наблюдаемым методом фотоэлектронной спектроскопии. Рассмотрена адсорбция атомов H, Cl и Ag на (111)-поверхности кремния. Основываясь на расчетах системы $Si_{13}H_{15}+Ag_7$ сделан вывод, что атомы серебра локализованы на атомах кремния, а не между ними.

И. Сенченя

Si_5 1982

Электрон.
строение,
теорет.
расчет.

Liebman Joel F.
Vincent James S.

Angew. Chem., 1982,
94, N 8, 649.

(см. $Li_{12}Si_7$; III)

Si_5

1984

3 Б1027. Расчет электронной структуры и плотности состояний идеальных и разупорядоченных кластеров кремния. Грехов А. М., Гунько В. М., Клапченко Г. М., Цященко Ю. П. «Теор. и эксперим. химия», 1984, 20, № 4, 477—488 (рус.)

В рамках кластерного приближения и методов ППДП/2, ЧПДП и МЧПДП/3 изучена электронная структура и плотности состояний кластеров Si_5 и Si_5H_{12}, моделирующих фрагменты реальной структуры объемного кремния, а также обсуждены изменения в электронной структуре кремния при топологич. разупо-

структура, геометрия

(41) IX

Х. 1985, 19, N3.

рядоченности решетки. Показано, что насыщение границ кластера атомами водорода уменьшает неоднородность в распределении электронной плотности и насыщающие атомы водорода можно считать аналогом внешнего по отношению к остову атомов Si самосогласованного Пт, имитирующего крист. окружение. Наиболее чувствительным к положению граничных атомов H оказывается средний пик «валентной зоны», к-рый смещается на 5 эВ, а наименее чувствительными — пик «валентной зоны» в области —28 эВ и дно «зоны проводимости». С увеличением длины связи Si—H ширина «запрещенной зоны» уменьшается. Все использованные методы дают порядок уровней «валентной зоны», согласующийся с данными неэмпирич. расчетов. Показано, что основное изменение ширины «запрещенной зоны» при разупорядочении обусловлено смещением дна «зоны проводимости». И. Н. Сенченя

1984.

Si_n

(n=2, 3, 5, 17 и 29)

1 Б1054. Кластерные расчеты для оценки зарядового распределения и гибридизации в кластерах Si. Cluster calculations for the investigation of charge distribution and hybridization in Si clusters. Weinert C. M. «Surface Sci.», 1985, 156, № 2: Small Part. and Inorg. Clusters. Proc. 3rd Int. Meet., Berlin (West), 9—13 July, 1984. Pt 2, 641—648 (англ.)

Методом ППДП проведены расчеты систем Si_n ($n=2$, 3, 5, 17 и 29). В кач-ве меры гибридизации атома Si использована величина $f=\Sigma_\mu P_{\mu\mu}/\Sigma_\nu P_{\nu\nu}$, где индекс μ пробегает по всем p-АО атома, а ν — по всем s-АО того же атома. Рассмотрено изменение f с ростом n (для изолированного атома $f=1$, в объемном Si $f=3$). Сопоставление электронного распределения, величины f и энергий в расчете на 1 связь для кластеров и объемного Si показало, что поверхн. эффекты в Si очень велики и доминируют над объемной частью. Найдено, что кластеры можно стабилизировать, если допустить релаксацию поверхн. части, минимизируя полную энергию. В кач-ве др. схемы построения больших кластеров указано построение их не из атомов, а из тетраэдрич. ячеек. М. Б. Кузьминский

расчет

Х·1986, 19, N1

$Si_n^{-(+)}$ (Ом. 23261) 1985

Bloomfield L.A., Geusic M.E.,
et al.,

структура

Chem. Phys. Lett.,
1985, ● 121, N 1-2,
33-37

Si_x^+

Ом·23821

1985

$x \leq 14$

103: 112766f **Mass spectra of silicon, germanium, and tin clusters.** Martin, T. P.; Schaber, H. (Max Planck Inst. Festkoerperforsch., 7000 Stuttgart, 80 Fed. Rep. Ger.). *J. Chem. Phys.* 1985, 83(2), 855-8 (Eng). Clusters of Group IV B elements were produced and obsd. in a mass spectrometer. Irregularities in the ion intensities identify clusters with particularly high or low stability. For example, Si_x^+, Ge_x^+, and Sn_x^+ show an enhanced stability for $x = 6, 10$. However, Sn_{14}^+ is unstable, whereas Ge_{14}^+ is particularly stable.

(стабильн.

(масс спектр.)

исследов.

Ge_x^+, Sn_x^+

(+2) IX

$x \leq 14$

С.А. 1985, 103, N 14.

Si_n^+

Оп. 23875

1985

$n = 7-45$

масспектр,
стабильн.

Phillips J.C.,

J. Chem. Phys., 1985,
83, N7, 3330-3333.

Si_n (n=2-7, 10) ОМ · 23390 1985

Si_n^+ (n=2-6)

13 Б1020. Структура и химическая связь в малых кластерах кремния. Structure and bonding in small silicon clusters. Raghavachari Krishnan, Logovinsky Veronika. «Phys. Rev. Lett.», 1985, 55, № 26, 2853—2856 (англ.)

Неэмпирическим методом ССП МО в базисе 6—31ГФ* проведены расчеты электронного и геометрич. строения нейтральных Si_n ($n=2—7$, 10) и ионных Si_n^+ ($n=2—6$) кластеров. Энергии кластеров уточнены с учетом электронной корреляции по теории возмущения Мёллера—Плессета 4-го порядка. Найденные геометрич. х-ки нейтр. кластеров существенно отличаются от геометрии микрокристаллов кремния. Рассчитанные Пт ионизации и энергии связи использованы для интерпретации распределения и фрагментации малых кластерных ионов кремния.

И. Н. Сенченя

структура

(Н) ☒

Х. 1986, 19, N 13

Si_n^+ (n=2-6)

Si_n
Si_n^+
$n = 2 - 7, 10$

Om. 23390

1985

104: [illegible]175h **Structure and bonding in small silicon clusters.** Raghavachari, Krishnan; Logovinsky, Veronika (AT & T Bell Lab., Murray Hill, NJ 07974 USA). *Phys. Rev. Lett.* 1985, 55(26), 2853-6 (Eng). Accurate ab-initio MO calcns. were done to obtain the ground-state geometries and electronic configurations of the silicon clusters Si_n for *n* = 2-7, 10, and Si_n^+ for *n* = 2-6. The effects of polarization functions and electron correlation were included in these calcns. All the optimized structures were considerably reconstructed from those derived from microcrystal geometries. Ionization potentials and binding energies were calcd., and used to interpret the obsd. (L. A. Bloomfield, et al., 1985) distribution and fragmentation of small silicon cluster ions.

структурн. параметры, энергии связи

④ ☒ Si_n^+ ● $(n = 2 - 6)$

C.A. 1986, <u>104</u>, N6

Si_n

1985

103: 129293x **Cluster calculations for the investigation of charge distribution and hybridization in silicon clusters.** Weinert, C. M. (Inst. Theor. Festkoerperphys., Freie Univ. Berlin, D-1000 Berlin, 33 Fed. Rep. Ger.). *Surf. Sci.* 1985, 156(2), 641–8 (Eng). Cluster calcns. using the semiempirical CNDO scheme were performed for clusters of 2, 3, 5, 17 and 29 Si atoms. The electronic distribution in the cluster, the hybridization and the bond charges were investigated and compared to cryst. bulk material. The large surface effects prevent small Si clusters to have bulk properties. Surface reconstruction of the clusters can increase central hybridization and binding energy per bond. Possible schemes for constructing larger Si clusters are derived.

структура
и электр.
св-ва клас
теров.

C. A. 1985, 103, N 16.

Si_n (Ст. 24396) 1986

$n \geq 2$ Koutecky J., Fantucci P.,

теорет.
расчет
структ.
и энергет.

Chem. Rev., 1986, <u>86</u>, N3, 539–587.

Si_n

От. 23761

1986

$(n = 3 \div 7)$

(теор. расчет)

(Н) ☒

104: 156193s Silicon and germanium clusters. A theoretica study of their electronic structures and properties. Pacchi Gianfranco; Koutecky, Jaroslav (Inst. Phys. Chem., Freie Un Berlin, 1000 Berlin, 33 Fed. Rep. Ger.). *J. Chem. Phys.* 1986, 84 3301-10 (Eng). Si and Ge clusters contg. 3-7 atoms were stud with the pseudopotential MO-LCAO method followed by C procedure. These clusters have very similar electronic structures an consequently analogous physicochem. properties but differ substantially from small C clusters. Linear structures are clearly less favorable than more compact structures. On the other hand, some planar geometries possess considerable stability. The Si and Ge clusters which are sections of the diamond-type crystal lattice are less stable than clusters which can be considered as segments of closed-packed lattices or as steps in pentagonal crystal growth. The reason is that the majority of atoms in small clusters are surface atoms which cannot assume the tetrahedral coordination characteristic of Si and Ge bulk atoms. The appearance of typical bulk properties is expected only for very large Si and Ge clusters with small surface atoms/bulk atoms ratio.

С. А. 1986, 104, N 18.

Ge_n

$Si_{\widehat{n}}$ 1986

(n = 3–7, 10) Raghavachari Krishnan.

ш.п.

J. Chem. Phys., 1986, $\underline{84}$, N 10, 5672–5686.

(см. Si_2; $\underline{\widehat{III}}$)

Si_6

1986

теор. расчет структуры

105: 121175f **LCAO-Xα-force study on stable structures of silicon Si_6 and Si_{10} clusters.** Saito, Susumu; Ohnishi, Shuhei; Satoko, Chikatoshi; Sugano, Satoru (Fund. Res. Lab., NEC Corp., Kanagawa, Japan 213). *J. Phys. Soc. Jpn.* **1986**, 55(6), 1791–4 (Eng). Stable structures of the Si_6 and the Si_{10} microclusters were calcd. by using the LCAO-Xα-force method. The calcd. structures of the Si_6 and the Si_{10} clusters resemble a regular octahedron and a tetrahedron, resp. In both clusters, triangles, consisting of the (111)-surface atoms of cryst. silicon, contract by 20% in length compared to those of the crystal. This contraction was attributed to the interaction between dangling bonds, and is important for silicon microclusters of any size.

(A1) ☒ Si_{10}. ●

C:A·1986, 105, N14

Si_n | От. 24699 „а" | 1986

$(n=2-7,10)$

Raghavachari K.,

J. Chem. Phys., 1986,
<u>84</u>, N10, 5672-5686.

теор.
расчет
структ.
и энер.

●

(См. Si_2, III)

Si_n От. 23699 1986

$n \leq 7$

лазерное испарен., масс-спектр.

Reents W.D., Bondybey V.E., Chem. Phys. Lett., 1986, ● <u>125</u>, N 4, 324-327.

Кластеры Si 1986

Yamanouchi Kaoru.

Nippon Butsuri Gakkai-shi 1986, 41 (11), 912-15.

(см. ● C_{60} ; III)

Si_{10} 1986

Saito Susumu,
Ohnishi Shuhei, et al.

теор. расчёт структ.

J. Phys. Soc. Jpn. 1986, 55(6), 1791-4.

(см. Si_6 ; III)

Si_n^- (От. 27242) 1987

(n=3-7)

Cheshnovsky O., Yang S.H., et al.,

фотоэл. спектр

Chem. Phys. Lett., 1987, <u>138</u>, N2-3, 119-124.

Si_n

$n=4,6,10$

1987

110: 13821h **Fragmentation of silicon microclusters.** Feuston, B. P.; Kalia, R. K.; Vashishta, P. (Argonne Natl. Lab., Argonne, IL 60439 USA). *NATO ASI Ser., Ser. B* **1987**, 158(Phys. Chem. Small Clusters), 283-8 (Eng). A detailed study of Si_n (n = 2–14) clusters has been performed through mol. dynamics (MD) simulation and the method of steepest descent quench (SDQ) with the Stillinger–Weber three-body potential. The approach is intrinsically a finite-temp. method which investigates all underlying mech. stable structures visited by the system in the equil. state. Results indicate that the magic nos., relatively stable clusters Si_N(n = 4,6,10), are detd. by the topol. and energetics of high energy bound structures rather than the structure and ground state energies at zero temp.

стабилн., теорет. расчет

C.A. 1989, 110, N2

Si_n

1987

$n = 2 \div 14$

(теор. расчет)

107: 121461n **Fragmentation of silicon microclusters: a molecular-dynamics study.** Feuston, B. P.; Kalia, R. K.; Vashishta, P. (Dep. Phys., Univ. Cincinnati, Cincinnati, OH 45221 USA). *Phys. Rev. B: Condens. Matter* 1987, 35(12), 6222–39 (Eng). A detailed mol.-dynamics study was performed to (*i*) enumerate ground-state and finite-temp. structures, and (*ii*) investigate the nature of fragmentation for Si_N clusters ($N = 2–14$), by using the Stillinger–Weber three-body interaction potential. All underlying mech. stable structures, visisted by the system in the equil. state, were studied. The presence of magic nos., unusually stable finite-temp. clusters Si_4, Si_6, and Si_{10} as detd. by the photofragmentation expt. of L. A. Bloomfield, et al., (1985), is dependent upon the topol. and energetics of high-energy bound structures, rather than upon the structure and ground-state energies at zero temp.

C. A. 1987, 107, N 14

$Si_{\widehat{m}}$

$m = 3 \div 7$

1987

Pacchioni Gianfranco,
Koutecky Jaroslav.

NATO ASI Ser., Ser. B
1987, <u>158</u>, 439–44.

эл.
структ.

●

(См. $C_{\widehat{n}}$; $\underline{\widehat{III}}$)

Si_n (От. 27684) 1987

$Si_n^{+,-}$

Phillips J.C.,

структура, теор. расчет J. Chem. Phys., 1987, <u>87</u>, N 3, 1712-1716.

$\mathrm{Si}_{\bar{п}}$ 1987

Pruett J. G., Windischmann H., et al.

лазерное испарение

NATO ASI Ser., Ser. B 1987, <u>158</u>, 109-14.

(см. $\mathrm{Ge}_{\bar{п}}$; <u>III</u>)

$Si_{\overset{\frown}{п}}$ 1987

Brown W. L., Freeman R. R., et al.

обзор Science, 1987, <u>235</u>, N 4791, 860-865.

(Сеег. ● $С_{\overset{\frown}{п}}$; $\underline{\overset{\frown}{III}}$)

Si_n 1987

107: 141539x **Structure and bonding of small semiconductor clusters.** Tomanek, D.; Schluter, M. A. (Dep. Phys., Univ. California, Berkeley, CA 94720 USA). *Phys. Rev. B: Condens. Matter* 1987, 36(2), 1208–17 (Eng). The geometrical and electron structure of small Si_n, Si_n^+, and Si_n^- clusters was calcd. up to $n = 14$ within a combined tight-binding-d.-functional-theory scheme. Esp. stable structures for $n = 6$ and 10 coincide with obsd. abundances in the exptl. mass spectra. All equil. structures are close packed, with a different bonding than in the bulk fragments. A transition to bulklike open structures occurs at $n \approx 10^2$–10^3.

структура,
теор. расчет

(+2) ☒ Si_n^+, Si_n^-

C.A. 1987, 107, N 16

Si_n^+

1987

Tomanek D., Schluter M.A.

струк-
тура,
теор.
расчёт.

Phys. Rev B: Condens. Matter 1987, <u>36</u> (2), 1208-17.

●

(см. Si_n^+; III)

Si$_{\overline{п}}$.

1987

Tomanek D., Schluter M. A.

структура, теор. расчёт

Phys. Rev B: Condens. Matter. 1987, $\underline{36}$ (2), 1208–17.

(см. Si$_{\overline{п}}$; $\overline{\underline{\text{III}}}$)

SiN

От. 28764

1988

равновесн-
структура,
ab initio
расчет

Ballone P., Andreoni W., et al.,

Phys. Rev. Lett., 1988, 60, N4, 271–274.

Equilibrium structures

and Finite Temperature Properties of Silicon Microclusters from Ab Initio Molecular-Dynamics Calculations

Si_x О.М. 30839 1988

теорет. расчет стабильн.

109: 135346g **Transition from metallic to covalent structures in silicon clusters.** Chelikowsky, James R. (Dep. Chem. Eng. Mater. Sci., Univ. Minnesota, Minneaplis, MN 55455 USA). *Phys. Rev. Lett.* 1988, 60(25), 2669-72 (Eng). The structural properties of Si clusters are examd. to det. at what size clusters with covalentlike open structures become energetically more stable than those with metalliclike close-packed structures. By calcn. of the total energy of diamond and face-centered cubic fragments as a function of the no. of atoms, an est. of the "crit." cluster size is made. The est. is that for clusters of less than about 50 atoms, metallic structures are favored over covalent structures, with the inequality reversed for more than 50 atoms. This result agrees well with recent observations on the relative stability of Si_n^+.

С.А. 1988, 109, N 16.

Si_n (2)

1988

, 109: 176649b Calculation of the energy spectrum of a polyatomic silicon cluster containing transition element atoms by the scattered waves Xα method. Gurskii, L. I.; Smol'skii, V. P.; Tralie, I. E. (USSR). *Klastery v Gaz. Faze. Novosibirsk* 1987, 168–71 (Russ). From *Ref. Zh., Khim.* 1988, Abstr. No. 8B1044. Title only translated.

C.A. 1988, 109, N 20

Si_n Ом, 30879 1988

109: 197576r **Collision-induced dissociation of silicon cluster ions.** Jarrold, Martin F.; Bower, J. Eric (AT and T Bell Lab., Murray Hill, NJ 07974 USA). *J. Phys. Chem.* 1988, 92(20), 5702-5 (Eng). The results of a study of the collision-induced dissocn. of Si_n^+ (n = 6-26), by Ar at a collision energy of 5 eV are described. The dominant products are Si_6^+ or Si_7^+ for smaller clusters (n < 15) and arise from loss of seven or ten atoms from the larger clusters. The obsd. products are virtually identical with those found in recent photodissocn. expts., which indicates that dissocn. occurs on the ground-state potential surface in the photodissocn. studies. From an anal. of the product distributions, ions (Si_n^+) with n = 6, 7, 10, and 11 and neutrals (Si_m) with m = 6, 7, and 10 are identified as favored products. The collision-induced dissocn. probabilities show local min. at n = 11, 15, 19, and 23, suggesting that these clusters are particularly stable toward dissocn. These clusters appear particularly stable mainly because they cannot fragment into a combination (n + m) of favored products with the ion n = 6, 7, 10, or 11 and neutral m = 6, 7, or 10.

(диссоциац)

C. A. 1988, 109, N 22

Si_n 1988

$3 \le n \le 10$

теор. расчет (структура и энергет.)

110: 121769f Structure and properties of small silicon and aluminum clusters. Jug, Karl; Schluff, Hans Peter; Kupka, Hans; Iffert, Ruediger (Theor. Chem., Univ. Hannover, 3000 Hannover, Fed. Rep. Ger.). *J. Comput. Chem.* 1988, 9(8), 803-9 (Eng). Small Si_n and Al_n clusters (n = 3-10) were studied with the semiempirical MO method (MO) method SINDO1. For each n, various structures were optimized to det. the most stable structure. To obtain good qual. agreement with available ab initio calcns. d orbitals had to be omitted from the basis set. Both Si and Al tend to build three-dimensional structures rather than two- or one-dimensional structures, except for n = 3 or 4. The structure growth was studied by approaching various sites of stable structures with one or more atoms. Si and Al exhibit different structure growth, and consequently, different most-stable structures. Ionization potentials, HOMO-LUMO energy differences, binding energies per atom, and av. at. valencies are presented.

㊶ ☒ Al_n ● $3 \le n \le 10$

C.A. 1989, 110, N 14

Si_n (От. 28669) 1988

(n=2-10) Raghavachari K.,
Rohlfing C.,

энергии
связи,
геометр.

Chem. Phys. Lett.,
1988, 143, N5, 428-434.

●

Si_n ОМ. 30I/91 1988

$7 \le n \le 10$

(теорет-расчет)

109: 197615c **Bonding and stabilities of small silicon clusters: a theoretical study of Si_7–Si_{10}.** Raghavachari, Krishnan; McMichael Rohlfing, Celeste (AT and T Bell Lab., Murray Hill, NJ 07974 USA). *J. Chem. Phys.* 1988, 89(4), 2219-34 (Eng). Ab initio calcns. have been performed to study the structures and energies of intermediate-sized Si clusters (Si_n, n = 7–10). All geometries have been optimized at the Hartree-Fock (HF) level of theory with the polarized 6-31G* basis set. The harmonic vibrational frequencies have been evaluated at the HF/6-31G* level of theory. Electron correlation effects have been included by means of fourth order Moeller-Plesset perturbation theory. The most stable structure for Si_7 is a pentagonal bipyramid and the lowest energy calcd. structures for Si_8–Si_{10} correspond to capped octahedral or prismatic geometrical arrangements. The evolution of the cluster geometries with increasing size is discussed. Clusters contg. 4, 6, 7, and 10 atoms have been identified as "magic nos." for small Si clusters, both theor. and exptl. The hybridization and bonding in small Si clusters is discussed. The results are used to interpret the recent photoelectron spectra of neg. Si cluster ions.

C.A. 1988, 109, N22

Si_n^+

1989

$(n = 11-25)$

111: 240268x Chemical reactivity and covalent–metallic bonding of silicon ion(1+) (Si_n^+ (n = 11–25)) clusters. Chelikowsky, James R.; Phillips, J. C. (Minnesota Supercomput. Inst., Univ. Minnesota, Minneapolis, MN 55455 USA). *Phys. Rev. Lett.* 1989, 63(15), 1653-6 (Eng). Using our earlier thermodn. force field we have calcd. the equil. structures of medium-size Si_n clusters (n = 11-25). We find the very surprising result that beginning at n = 7, near n = 13 and near n = 19, these clusters follow a pentagonal growth pattern (icosahedra plus assocd. face capping). Our results are fully consistent with magic nos. recently found in the reaction rates for addn. of first C_2H_4 mols. to Si_n^+ clusters.

стабильн.,
расчёт

C.A. 1989, 111, N 26

Si_8

1989

111: 240188w Geometries and stabilities of silicon (Si_8) clusters. Kupka, H.; Jug, K. (Univ. Hannover, D-3000 Hannover, Fed. Rep. Ger.). *Z. Phys. D: At., Mol. Clusters* 1989, 13(4), 301-6 (Eng). The relative stabilities of eight-atom Si clusters were calcd. with the semiempirical MO method SINDO1. With the aid of the group theor. concept of kernels and epikernels, stationary points of D_{2d}, C_{2v} and C_s symmetry on the potential energy surface near the unstable cube were found. Part from these stationary points which adopt epikernel symmetries, a D_{4d} stationary point not derivable from group theory is possible in configuration space. The cubic array with eight equiv. with eight atoms can be classified as a diradical.

расчет

C.A.1989, 111, N26

Si_8

1989

3 Д47. **Геометрия и стабильность кластеров Si_8.** Geometries and stabilities of Si_8 clusters / Kupka H., Jug K. // Z. Phys. D.— 1989.— **13**, № 4.— С. 301—306.— Англ.

С использованием полуэмперич. метода SINDO 1 и с применением теоретико-группового подхода (ТГП) изучены поверхности потенц. энергии (ППЭ) для различных конформеров кластера Si_8. Для полученных ППЭ исследованы стационарные точки (СТ), в том числе СТ для переходных состояний. Найдено, что структура (8, 18, 12), соответствующая наиболее симметричному графу, является энергетически наиболее выгодной и отвечает деформированному додекаэдру симметрии C_s. Отмечено, что ТГП не позволяет определить все имеющиеся СТ, напр. не определяется СТ симметрии D_{4d}. Указано, что кубич. кластер Si_8 является нестабильным и ведет себя, как дирадикал.

А. И. К.

М.Л.

ф. 1990, №3

Si_n

1989

$n>6$

110: 141868r **Potential model for silicon clusters.** Mistriotis, A. D.; Flytzanis, N.; Farantos, S. C. (Dep. Phys., Univ. Crete, Heraklio, Greece GR-711 10). *Phys. Rev. B: Condens. Matter* 1989, 39(2), 1212–18 (Eng). An interat. potential for Si is proposed, which is a significant improvement over the Stillinger–Weber model. This potential is valid for clusters with more than six atoms, where π bonding is not significant because of the large degree of coordination. Guided by ab initio electronic calcns., the authors introduced four-body interactions to the potential, which were essential to give good agreement with the m.p. of the crystal and the geometries and the energies of the ground and low metastable states of silicon clusters.

теор.
расчет

C.A. 1989, 110, N 16

Si_n Кластеры 1989

Si_n^+, Si_n^- Raghavachari
Krishnan.

кв. мех.
расчёт

Z. Phys. D: At, Mol.
Clusters 1989, <u>12</u>(1-4),
61-4.

(См. Кластеры C_n; III)

Кластеры
Si_N
($N=2-7$)
колебат-
св-ва,
Тт

От. 31595

1989

Li Jian Zhang Kai-ming.,

Acta Phys. Sinica, 1989, 38, N 2, 343-348.

The Vibrational Properties

and Melting Temperatures
of Small Si Clusters.

Si_4^- (ОМ 35380) 1990

Kitsopoulos T.N., Check C.J., et al.,

J. Chem. Phys., 1990, 93, N8, 6108–6110.

Vibrationally resolved photoelectron spectra of Si_3^-

and Sig.

Si_{10}

1990

115: 57438w **Electronic and structural properties of silicon 10 cluster.** Rantala, T. T.; Jelski, D. A.; George, T. F. (Dep. Chem., State Univ. New York, Buffalo, NY USA). *Report* 1990, UBUF=FALO/DC/90/TR-12; Order No. AD-A222429. 26 pp. (Eng). Avail. NTIS. From *Gov. Rep. Announce. Index (U. S.)* 1990, 90(19), Abstr. No. 047,491. Possible structures for Si_{10} cluster are considered using a tight-binding model and drawing on significant work done in the past. The tight-binding parametrization, fitted to the bulk, is also valid for smaller systems. This model is found to essentially reproduce other published results, but requires much less effort than ab initio techniques, thus allowing the study of a wide variety of structures and their ions. However, unlike classical force field calcns., it yields information about the electronic structure of clusters. A new geometric structure for Si_{10} is found, which is not only of lowest energy, but which also matches the exptl. photoelectron band gap and explains the exptl. reactivity data. Because of the Jahn-Teller effect, the photoelectron spectrum is very sensitive to geometry. Also, ionization of the cluster alters the geometry slightly.

геометрия,
структура,
расчет

C.A. 1991, 115, N6

Si_n

$(n=2\div10)$

1990

113: 46751a A theoretical study of small silicon clusters using an effective core potential. Rohlfing, Celeste McMichael; Raghavachari, Krishnan (Theor. Div., Sandia Natl. Lab., Livermore, CA 94551-0969 USA). *Chem. Phys. Lett.* **1990,** 167(6), 559–65 (Eng). The structures and energies of small Si clusters are investigated using an effective core potential (ECP), a double-zeta polarized basis set, and fourth-order Moeller-Plesset perturbation theory. Excellent agreement is obtained with the results of recent all-electron calcns. for Si_2–Si_{10}. The ECP is used to examine Si_{11}, which has not been previously characterized. The lowest-energy structure of Si_{11} is found to be a distorted pentacapped trigonal prism, which offers further growth possibilities.

структура,
стабильност,
расчет

C.A. 1990, <u>113</u>, N6

Si_6 1991

теор. расч., стабильн.

Al-Laham M.A.; et al.,
Chem. Phys. Lett.,
1991, 187(1-2), 13-20

(см. fabs ●; III)

$Si\overset{\frown}{n}$ 1991

$n = 3-7$

Erkoc S.

структура, До, расчет

Z. Phys. D: At., Mol. Clusters 1991, 19(1-4), 423-5.

(см. ● $C\overset{\frown}{n}$ $n=3-7$; III)

Si_n

1991

теорет. расчет
стабильности
кластеров и
структур. перех

116: 28499g Silicon cluster ions: evidence for a structural transition. Jarrold, Martin F.; Constant, Vladimir A. (AT and T Bell Lab., Murray Hill, NJ 07974 USA). *Phys. Rev. Lett.* 1991, 67(21), 2994–7 (Eng). The mobilities of size-selected silicon cluster ions in helium have been measured using injected-ion drift-tube techniques. A major structural transition occurs for clusters with ~27 atoms. Clusters with up to ~27 atoms appear to follow a prolate growth sequence, resulting in geometries with an aspect ratio estd. to be ~3. Larger clusters appear to have more spherical shapes. For annealed clusters this structural transition occurs over a narrow size range.

С.А. 1992, 116, N 4

Si_{45}

1991

118: 220126r **Structure of the silicon (Si_{45}) cluster.** Jelski, D. A.; Swift, B. L.; Rantala, T. T.; Xia, X.; George, T. F. (Dep. Chem., Washington State Univ., Pullman, WA USA). *Report* 1991, WSU-DC/91/TR-61; Order No. AD-A240278, 32 pp. (Eng). Avail. NTIS. From *Gov. Rep. Announce. Index* (*U. S.*) 1992, 92(1), Abstr. No. 200,379. There has been much interest in the Si cluster, both from an exptl. and theor. point of view. The original impetus to this effort was the astounding exptl. results compiled by Elkind et al, which reported a reactivity difference between various Si clusters spanning two orders of magnitude. Silicon ions were found to be unreactive with ammonia and methanol. This implied a periodicity of six atoms in the reactivity pattern for clusters ranging form 30 to 45 atoms. For clusters larger than 45 atoms the reactivity appeared to monotonically increase. J. C. Phillips suggested that Si forms six-membered rings in a carbon-like fashion and proposed a structure of stacked ring with a three-atom cap. We took this suggestion literally, and in what we believe to be the first calcn. which tried to explain this data, proposed a series of stacked benzene rings and attempted to show that this accounted for the expt.

теорет.
(расчет
кластеров)

C.A. 1993, 118, N 22

Si_{45}

1991

117: 34022h Structure of the silicon forty-five-atom cluster. Jelski, Daniel A.; Swift, Brian L.; Rantala, Tapio T.; Xia, Xinfu; George, Thomas F. (Coll. Fredonia, State Univ. New York, Fredonia, NY 14063 USA). *J. Chem. Phys.* 1991, 95(11), 8552-60 (Eng). Six structures for the Si_{45} cluster are compared using a tight-binding model. Two new structures are proposed which appear to be the low-energy isomers and to explain much of the existing exptl. data. Cluster reactivity is distinguished from cluster stability, and several reasons are discussed which may lead to a reactive or unreactive species. These criteria are applied to the Si_{45} isomers, and the results are also correlated with exptl. data.

(структура)

C. A. 1992, 117, N4

Si_n

1991

$(n=2 \div 10)$

115: 79253j **Electronic structures of the negative silicon cluster ions (Si_2^-–Si_{10}^-): electron affinities of small silicon clusters.** Raghavachari, Krishnan; Rohlfing, Celeste McMichael (AT and T Bell Lab., Murray Hill, NJ 07974 USA). *J. Chem. Phys.* 1991, 94(5), 3670–8 (Eng). Accurate ab–initio calcns. have been performed to investigate the structures and energies of the neg. ions of Si_2–Si_{10}. The effects of polarization functions, diffuse functions, and electron correlation have been included in these calcns. In most cases, there is a good correspondence between the ground–state structures of the neg. ions and those of the corresponding neutral species. Adiabatic electron affinities are computed and compared with recent exptl. measurements. Si_3, Si_5, Si_8, and Si_9 are found to have electron affinities which are larger than their neighbors. This result is interpreted using our previous calcns. (C. M. R. and K. R., 1990) on the low–lying states of the corresponding neutral species.

структура, электрон. состоян., расчет

C.A. 1991, 115, N8

Si_5^-

1992

116: 91876t **Stable and metastable states of the silicon pentaatomic mononegative ion. Theoretical study.** Adamowicz, Ludwik (Dep. Chem., Univ. Arizona, Tucson, AZ 85721 USA). *Chem. Phys. Lett.* 1992, 188(1-2), 131-4 (Eng). The Si_5^- cluster forms a bitrigonal pyramid. This structure can form some stable and metastable (autodetaching) states with an addnl. electron, which attaches to the cluster surface. Energies of some of those states are detd. based on ab-initio calcns. with the use of the coupled-cluster method combined with the first-order correlation orbital method. It is found that at least four states, i.e., X^2A_2'', $^2E'$, $^2E''$, and $(2)^2E'$, lie below the electron ejection threshold.

теорет.
расчет
стабильн. и
структура

C.A. 1992, 116, N 10

Si_5^-

1992

6 Д180. **Стабильные и метастабильные состояния аниона Si_5^-. Теоретические исследования.** Stable and metastable states of the Si_5^- anion. Theoretical study / Adamowicz Ludwik // Chem. Phys. Lett.— 1992.— 188, № 1—2.— С. 131—134.— Англ.

Кластеры Si_5 имеют структуру битригональной пирамиды. Эта структура может создавать стабильные и метастабильные (автоотрывные) состояния с дополнительным электроном, который прилипает к поверхности кластера. Определены энергии некоторых из этих состояний. Применялся метод связанных кластеров в комбинации с методом орбитальной корреляции первого рода. Получено, что по крайней мере 4 состояния (X^2A_2'', $^2E'$, $^2E''$ и $(2)^2E'$) лежат ниже порога отрыва электрона. Приводятся сопоставления с эксперим. данными. В связи с большой ненасыщенностью поверхности кластера очень велика вероятность прилипания электрона к кластеру. В масс-спектральных экспериментах наблюдались соответствующие стабильные анионы.

И·Л·

сф. 1992, N6

Si_n, Si_n^- (Ом. 37401) 1992

$n = 1 \div 5$

Энергии связи,
Ae,
теор. расчёт

117: 14684x **Binding energies and electron affinities of small silicon clusters (n = 2-5).** Curtiss, Larry A.; Deutsch, Peter W.; Raghavachari, Krishnan (Cehm. Technol. Div., Argonne Natl. Lab., Argonne, IL 60439-4837 USA). *J. Chem. Phys.* **1992**, 96(9), 6868-72 (Eng). The Gaussian-2 (G2) theory procedure, based on ab initio MO theory, is used to calc. the energies of Si_n and Si_n^- (n = 1-5) clusters. The G2 energies are used to derive accurate binding energies and electron affinities of these clusters. The calcd. electron affinities of Si_2-Si_4 are in agreement to within 0.1 eV with results from recent photoelectron spectroscopic measurements.

C.A. 1992, 117, N2

Si_n

1992

$5 \leq n \leq 12$

118: 198679z Structure and dynamics of silicon. Flytzanis, N.; Mistriotis, A. D.; Vendras, P. J. (Dep. Phys., Univ. Crete, Heraklio, Greece 71409). *J. Mech. Behav. Mater.* 1992, 4(1), 41–50 (Eng). The authors developed an interat. potential for Si for Monte Carlo or mol.-dynamic simulations which is an improvement of the Stillinger–Weber (SW) potential, including 4-body terms in a weighted way. Calcns. give very good agreement for the energy and structure of the ground states of the cluster Si_n ($5 \leq n \leq 12$) compared with ab initio electronic calcns. The fragmentation process of Si clusters was studied. The model was used to calc. bulk elastic consts. in reasonable agreement with exptl. data. Results on the amorphous structure are also reported.

структура
и энергетика

C. A. 1993, 118, N 20

Si_{10}

1992.

структура, хим. связь, теор. расчет

117: 14687a Long bonds in silicon clusters: a failure of conventional Moeller-Plesset perturbation theory? Messmer, Richard P.; Patterson, Charles H. (Gen. Electr. Corp. Res. and Dev. Cent., Schenectady, NY 12301 USA). *Chem. Phys. Lett.* **1992**, 192(2-3), 277-82 (Eng). On the basis of generalized valence bond calcns. the authors propose a new type of structure for the Si_{10} cluster. This structure is found to have intra-pair correlation effects, suggesting the inadequacy of a single determinant ref. wave function in conjunction with Moeller-Plesset perturbation theory for detg. the relative energetics of silicon clusters. The bonding in Si_{10} is analyzed and the origin of the large intra-pair correlation effects is found to be four "long bonds" in the new Si_{10} geometry.

С. А. 1992, 117, N2

Si_{10}

1992

118: 87941j **Structures of Si_{10}. Are there conventionally bonded low-energy isomers?** Raghavachari, Krishnan; Rohlfing, Celeste McMichael (AT&T Bell Lab., Murray Hill, NJ 07974 USA). *Chem. Phys. Lett.* **1992**, 198(5), 521–5 (Eng). Accurate quadratic configuration-interaction calcns. including the effects of triple excitations were performed on different isomers of Si_{10}. In agreement with previous studies, a tetracapped trigonal prism (C_{3v}) is slightly more stable (0.3 eV) than a tetracapped octahedron (T_d). Both these compact structures involving polyhedral bonding are considerably more stable (2.5 eV) than a conventional tetrahedrally bonded D_{2h} structure proposed recently by Messmer and Patterson. In addn., the D_{2h} isomer is not a local min. and collapses to a polyhedrally bonded C_{2h} structure which is 1.6 eV less stable than the C_{3v} form.

структура, теор. расч.

C.A. 1993, 118, N10

Si_{13} 1992

Roethlisberger U.,
Andreoni W., et al.,

структура,
теор.
расчет

J. Chem. Phys., 1992,
96 (2), 1248–56.

(см. Na_{13}; ● III)

Si_n Om 36856 1992

$n=3-7$ Von Niessen W., Zakrzewski V.G.,

Ber. Bunsenges. Phys. Chem.
1992, <u>96</u>, N9, 1228 - 1232.

Ae

Complex Electron Affinity
Processes in Clusters of S
and Si.

Si_4, Si_4^+

1993

119: 281377r Study of silicon tetraatomic molecule and monopositive ion (Si_4 and Si_4^-) using threshold photodetachment (ZEKE) spectroscopy. Arnold, Caroline C.; Neumark, Daniel M. (Dep. Chem., Univ. California, Berkeley, CA 94720 USA). *J. Chem. Phys.* **1993**, 99(5), 3353–62 (Eng). The threshold photodetachment (ZEKE) spectrum of Si_4^- is presented. Although no transitions to the ground state of Si_4 are obsd., the authors obtain detailed information on the anion and several of the low-lying excited states of neutral Si_4. The spectrum shows a long progression of well-resolved transitions between the D_{2h} $^2B_{2g}$ rhombus anion and ν_2 vibrational levels of the first excited D_{2h} $^3B_{3u}$ neutral. The length and spacing of the progression is consistent with ab initio calcns. performed by Rohlfing and Raghavachari [J. Chem. Phys. 96, 2114 (1992)], but some of the sequence bands obsd. within the progression are not. The authors also observe transitions to the Si_4 $^1B_{3u}$ state which is found at a lower excitation energy than predicted. The perturbed vibrational structure in this band is attributed to vibronic coupling to a nearby electronic state which is "dark" with respect to ZEKE spectroscopy. The ZEKE spectra are compared to the previously obtained photoelectron spectra of Si_4^- as well as ab initio calcns. on Si_4^- and Si_4.

спектр,
структура

C.A.1993, 119, N 26

Si_n

1993

$n=2 \div 40$

119: 234514y **Photoionization of small silicon clusters: ionization potentials for silicon clusters Si_2 to Si_{40}.** Fuke, K.; Tsukamoto, K.; Misaizu, F. (Inst. Mol. Sci., Okazaki, Japan 444). *Z. Phys. D: At., Mol. Clusters* 1993, 26(Suppl.), 204-6 (Eng). Photoionization thresholds of Si_n (n = 2-40) were examd. by vacuum UV radiation (5.7-8.5 eV) generated by stimulated Rman scattering of narrow-bandwidth 193-nm radiation in high pressure hydrogen and deuterium gases. A strong threshold energy dependence on cluster size is obsd., featuring major max. at 10 and 20. The magic behavior at n=10 is consistent with the results of the photofragmentation and CID expts. reported previously.

Фотоионизация —
[illegible], I

C.A. 1993, 119, N22

Si_6

1993

119: 15511s **Density-functional study of the bonding in small silicon clusters. [Erratum to document cited in CA117(18):178529b].** Fournier, Rene; Sinnott, Susan B.; DePristo, Andrew E. (Ames Lab., USDOE, Ames, IA 50011 USA). *J. Chem. Phys.* **1993**, 98(11), 9222 (Eng). Errors related to the labeling of clusters and to the bond lengths in Figs. 2 and 4, Table I, subsection Si_6, and the caption of Table IV have been cor. The errors were not reflected in the abstr. or the index entries.

теорет-
расчет
структуры,
стат-поправка

C-A-1993, 119, №2

Si_n
($n>10$)

1993

120: 15394b Quantal estimates of binding energies of large silicon clusters $(Si)_n$ with $n>10$. Oshiro, T.; Lutrus, C. K.; Hagen, D. E.; Beck, S.; Salk, S. H. Suck (Dep. Phys., Univ. Missouri, Rolla, MO 65401 USA). *Solid State Commun.* 1993, 87(9), 801–4 (Eng). The authors employ a computationally accessible semiempirical effective Hamiltonian method to calc. binding energies for large silicon clusters $(Si)_n$, for $n > 10$. The differences in binding energy between different geometric structures at a given cluster size generally tend to decrease with cluster size. This implies the possibility of cluster growth close to cryst. structure with Td symmetry at certain finite temps.

(Энергии связи)

теор. расчёт

C. A. 1994, <u>120</u>, N2

Si_{60}

1993

119: 256910b AM1 prediction of the equilibrium geometry of silicon cluster Si_{60}. Piqueras, M. C.; Crespo, R.; Orti, E.; Tomas, F. (Department of Physical Chemistry, University of Valencia, Dr. Moliner, 50, Burjassot, Valencia, Spain 46100). *Chem. Phys. Lett.* 1993, 213(5–6), 509–13 (Eng). AM1 calcns. have been carried out to det. the equil. geometry of Si_{60}. The predicted I_h geometry shows that bonds may be clearly identified as single (2.297 Å) or arom. (2.092 Å). Several analogies and differences between Si_{60} and C_{60} are pointed out. Esp. remarkable is the bigger size of the Si_{60} cluster, which is predicted to have a radius 2 Å larger than that of the C_{60} cluster. Results are compared to other levels of theory.

структура, расст.

C.A. 1993, 119, N24

Si_6, Si_{10}

1993

120: 331644u Study of Si_6 and Si_{10} microclusters with self-consistent-field and multi-scattering Xα method. Sun, Guoyao; Liu, Huizhou; Chen, Changyuan (Dep. Phys., Zhongshan Univ., Canton, Peop. Rep. China). *Zhongshan Daxue Xuebao, Ziran Kexueban* **1993**, 32(4), 119–23 (Ch). The mechanism of existing the magic no. of Si microclusters is analyzed by considering the dangling bonds. The possible structures of Si_6 and Si_{10} are studied by using the SCF and Xα scattered wave method and by taking into account the min. total energy of the clusters. Both the dangling bonds and the distortion of the bond angles play roles in Si microclusters.

(структура)

C.A. 1994, 120, N 26

Si_n
$n \leq 18$

1994

120: 227570f **A tight-binding molecular dynamics study of the equilibrium structures of small Si clusters.** Lee, In Ho; Chang, K. J.; Lee, Young Hee (Dep. Phys., Korea Adv. Inst. Sci. Technol., Daejon, S. Korea). *J. Phys.: Condens. Matter* 1994, 6(3), 741-50 (Eng). The authors present the results of tight-binding mol. dynamics calcns. for studying the equil. structures and the bonding properties of Si_n clusters for n up to 18. To prevent unphys. large charge transfer between different atoms in clusters, the authors employ the at. charge neutrality constraint that each atom has approx. four valence electrons. With a limited no. of parameters in the tight-binding scheme, the structures of min. energy are well reproduced, as compared with results from previous ab initio quantum mech. calcns. The authors find the abundant cluster sizes n = 4, 7 and 10, which are in good agreement with other theor. and exptl. results. For n ≥ 7, surface-like compact structures with a pentagon or a hexagon base are found to be energetically favorable, resulting in the metallic nature of the cluster bonding, while a core-based structure appears first for Si_{15}.

теор. рас
чет ста-
бильн. и
структура

C.A. 1994, 120, N18

Si_9 – Si_{16}

1994

121: 66081a Application of the many-body expansion potential energy functions to the study of Group IV atomic microclusters. (IV). Structures and stabilities of Si_9–Si_{16} microclusters. Li, Sidian (Dep. Chem., Yuncheng Adv. Train. Coll., Yuncheng, Peop. Rep. China 044000). *Gaodeng Xuexiao Huaxue Xuebao* 1994, 15(1), 108–12 (Ch). A many-body expansion potential energy function is used to study the structures and stabilities of Si microclusters, suggesting that firstly, Si_4–Si_{16} clusters can be constructed by successively adding 2- or 3-coordinated atoms, forming surfaces covered with 4-membered butterfly rings (D_{2d}); secondly, the trigonal bipyramid $Si_5(D_{3h})$ and D_{2d} Si_6 are the building blocks for most of these compact structures with a D_{4d} cage Si_{10} added in for the clusters with over 10 atoms and both Si_{10} and Si_{16} are covered with 3- or 4- or 5-coordinated atoms, predicting that Si_5, Si_6, Si_{10}, and Si_{16} be the prominent peaks in the mass spectra of fragmentized Si clusters, in agreement with expts.; and finally, these non-diamond compact structures have a max. coordination no. of 5 and the formation of 6-coordinated Si centers within half a sphere leads to destabilization in energy.

структура,
стабильн.,
теор. расчет

C. A. 1994, <u>121</u>, N6

Si$_{60}$

1994

теор. расчет структуры и стабильности

120: 227607y **Structure of Si$_{60}$. Cage versus network structures.** Menon, Madhu; Subbaswamy, K. R. (Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506-0055 USA). *Chem. Phys. Lett.* 1994, 219(3-4), 219-22 (Eng). A generalized tight-binding mol. dynamics technique which was used to obtain complete agreement with ab initio results for small silicon clusters is used to optimize the Si$_{60}$ cage without any symmetry restrictions. The perfect icosahedral cage is found to be unstable, distorting to a lower symmetry C_{2h} structure with no change in the threefold coordination. The relaxed geometry shows increasing tendency for tetrahedral arrangement of atoms, and is energetically unfavorable compared to a relaxed bulk-like fragment. This is in contrast to carbon, where the cage is favored.

C.A. 1994, 120, N18

$Si_{\widehat{60}}$ 1994

Slanina Z., Lee Shyi-Long.

(Датомиз.) Fullerene Sci. Technol. 1994, 2 (4), 459-69.

(См. $C_{\widehat{60}}$; II).

Si_n^{2-}

1994

$n = 5, 6, 11, 12$

120: 280567m **Electronic structure of small silicon clusters.** Wales, David J. (Univ. Chem. Lab., Cambridge, UK CB2 1EW). *Phys. Rev. A* 1994, 49(3), 2195–8 (Eng). Predictions by the tensor–surface–harmonic theory of A. J. Stone (1980–1, 1984) for bonding in small silicon clusters (Si_n^{2-}, n = 5, 6, 11, and 12) were tested by ab–initio calcns. Stable geometries, along with the energies and symmetries of the occupied MOs, can all be rationalized within the model. For example, local energy min. for the Si_n^{2-} clusters were found, which are isostructural with the borane and carborane clusters $B_nH_n^{2-}$ and $C_2B_{n-2}H_n$. In particular, both Si_{12}^{2-} and Si_{12}^{2+} exhibited icosahedral geometries, which were true min.

(ab initio расчет)

C. A. 1994, 120, N 22.

Si_n

1995

$n \leq 20$

(теор. расчет)

. 122: 197514n **Quantum Monte Carlo determination of electronic and structural properties of Si_n clusters ($n \leq 20$).** Grossman, Jeffrey C.; Mitas, Lubos (Dep. Phys., Univ. Illinois at Urbana-Champaign, Urbana, IL 61801 USA). *Phys. Rev. Lett.* 1995, 74(8), 1323-6 (Eng). Variational and fixed-node diffusion Monte Carlo methods are applied to study the structural and valence electronic properties of Si_n clusters. Binding energies for $n \leq 7$ agree within ≈4% with expts. and within ≈2% when the fixed-node error is decreased by using natural orbitals. For $n \geq 9$ we show that the local-d. approxn. overbinds by ≈25%. We detd. unambiguously (i) the role of correlation in the energy ordering for different structures, including our new lowest energy structure of Si_{20}, and (ii) a different ground state for Si_{13}^- than the one predicted by the local-d. approxn.

C. A. 1995, 122, N 16

Si_n

1995

$n = 4-7$

123: 211502m Vibrational modes of silicon nanostructures. Jing, Xiaodun; Troullier, N.; Chelikowsky, James R. (Minnesota Supercomputer Inst., Univ. Minnesota, Minneapolis, MN 55455 USA). *Solid State Commun.* 1995, 96(4), 231–5 (Eng). The authors present a method for predicting the vibrational modes of small semiconductor clusters. The authors employ ab initio pseudopotentials and apply a higher-order finite difference procedure to solve the Kohn–Sham equations. The authors predict the vibrational modes of small Si clusters (Si_n, n = 4–7) based on their ground state structures. The authors' calcd. vibrational modes agree very well with exptl. data, and with other theor. calcns. based on quantum chem. and tight binding methods. This comparison confirms the accuracy of the finite difference procedure for calcg. not only the 1st order deriv. of the energy, but the 2nd derivs. as well. It also validates the accuracy of pseudopotential–local d. calcns. for the ground state structures for Si clusters.

ab initio
(расчет)

C.A. 1995, 123, N 16

$Si_3 \div Si_7$ Om 38 009 1995

123: 240526c Si_3–Si_7. Experimental and theoretical infrared spectra. Li, S.; Van Zee, R. J.; Weltner, W. Jr.; Raghavachari, Krishnan (Department of Chemistry and Center for Chemical Physics, University of Florida, Gainesville, FL 32611-7200 USA). *Chem. Phys. Lett.* **1995,** 243(3,4), 275–80 (Eng). IR absorption bands in Ne, Ar, and Kr matrixes at 4 K were assigned to Si_3, Si_4, Si_6, and Si_7 from isotopic splittings and from ab initio calcns. of their vibrational frequencies and relative intensities. The agreement between exptl. and calcd. frequencies is excellent. Si_5 is apparently in too low a concn. to be obsd.

(ИК в матрице)

C.A. 1995, 123, N 18

Si_n
$n \leq 15$

1995

Nakajima A., Nakao K.
et al.
Mater. Res. Soc. Symp. Proc.
1995, <u>358</u>, 61-6.

(Ae)

● (см. Si_nNa ; $\underline{\overline{iii}}$)

Si_{70}

Оп 37828

1995

122: **197370n Electronic structure and bonding in Si_{70}.** Piqueras, M. C.; Crespo, R.; Tomas, F. (Dep. Quim. Fis., Univ. Valencia, Valencia, Spain E-46100). *J. Mol. Struct.* **1995**, 330, 177–80 (Eng). A detailed AM1 investigation is reported of the geometrical and electronic structure of Si_{70}. For this purpose, bond lengths, bond orders, charges and mol. energy levels are widely analyzed, and compared with previous theor. and exptl. data on Si_{60} and homologous carbon clusters C_{70} and C_{60}. The predicted D_{5h} structure of Si_{70} is less delocalized than that of C_{70}. Furthermore, Si_{70} presents the lowest ionization potential (7.63eV), the highest electron affinity (3.61 eV) and the smallest HOMO–LUMO gap (4.02 eV) of the four studied clusters.

I, Ae, структура и связь, теор. расчет.

C. A. 1995, 122, N 16

$Si_2 \div Si_7$ 1995

Raghavschari K.,
Curtiss L. A.

теор. расчёт

Understanding Chem.
React. 1995, <u>13</u>, 173-207.

(см. $C_2 \div C_7$; <u>III</u>)

Si_{46}

1995

123: 41280t **Electronic and structural properties of Si_{46}: a novel solid of silicon fullerenes.** Saito, Susumu; Oshiyama, Atsushi (Dep. Phys., Tokyo Inst. Technol., Tokyo, Japan 152). *Mater. Res. Soc. Symp. Proc.* 1995, 358(Microcrystalline and Nanocrystalline Semiconductors), 55–60 (Eng). The electronic structure is studied of the S_{46} lattice having 1nm-size unit cell using the d.-functional theory. The Si_{46} lattice consists essentially of dodecahedral-cage Si_{20} fullerenes proposed previously. Although all the Si atoms are tetrahedrally coordinated, the electronic structure is considerably different from that of the diamond Si lattice due to the pentagonal Si–Si network. Si_{46} is considered an important new Si semiconductor to be synthesized in the future. The authors also report the electronic structure of $Na_2Ba_6Si_{46}$. The mater. is metallic and the Fermi-level d. of states is very high due to the hybridization between Si and Ba states, which should be of essential importance for the supercond. obsd. in Na and Ba co-doped Si_{46}.

стр-ра
и
св-ва

C.A. 1995, 123, N4

Si_{24}) Si_{32} 1995

Stankevich I.V., Chistyakov A.L., et al.

теор. расчёт структ. парам., I, $\Delta_f H$

Zh. Strukt. Khim. 1995, $\underline{36}$ (6), 976-82. (см. $B_{\overline{n}}N_{\overline{n}}$; $\underline{iii}$)

1995

F: Si(n)
P: 3

8Б153. Расчет потенциалов ионизации небольших кластеров кремния методом сильной связи. Tight-binding calculation of ionization potentials of small silicon clusters / Zhao Jijun, Chen Xiaoshuang, Sun Qiang, Liu Fengqi, Wang Guanghou // Phys. Lett. A. - 1995. - 198, N 3. - С. 243-247. - Англ.

Методом локализованных орбиталей в приближении сильной связи рассчитаны потенциалы ионизации (ПИ) кластеров Si[x], x=2-12. Использованы геометрич. параметры, найденные в модели силового поля. Полученные результаты согласуются с эксперим. данными лучше, чем данные расчетов в приближении локальной плотности и в модели сферич. капли. Обнаружен локальный максимум ПИ для x=10, соответствующий магн. числу. Обсуждено влияние структурной изомеризации и релаксации кластеров на ПИ.

Х. N8, 1996

Si_n

$n \leq 20$

1995

122: 170707r Tight-binding calculation of ionization potentials of small silicon clusters. Zhao, Jijun; Chen, Xiaoshuang; Sun, Qiang; Liu, Fengqi; Wang, Guanghou (Department of Physics and National Laboratory of Solid State Microstructures, Nanjing University, Nanjing, Peop. Rep. China 210093). *Phys. Lett. A* 1995, 198(3), 243–7 (Eng). The size dependence of ionization potentials (IPs) of silicon clusters is studied using a localized orbital theory on the basis of the tight-binding approxn. The geometric structures of the silicon clusters are from the theor. results of the force field model, and the hopping integral and overlap integral in the tight-binding Hamiltonian matrix are obtained from the best fitted formula for the Slater–Koster parameters. It has been found that the present results conform to expts. much better than the previous LDA calcn. and the estn. of the spherical droplet model. The local max. of the IPs for Si_{10} is obtained, corresponding to the magic no. behavior obsd. by other exptl. means. The structural isomer effect and relaxation effect on the IPs of the silicon clusters are also discussed.

I, структура,
теор. расч

C. A. 1995, 122, N14

Si_{60}

1996

ab initio
расчет

124: 299395h Ab initio investigation of icosahedral Si_{60}. Crespo, R.; Piqueras, M. C.; Tomas, F. (Departament de Quimica Fisica, Universitat de Valencia, Dr. Moliner 50, Burjassot, Spain E−46100). *Synth. Met.* **1996**, 77(1−3), 13−15 (Eng). We present an ab initio all electron theor. investigation of the geometrical and electronic structures of icosahedral Si_{60}, using STO−3G, STO−3G*, 3−21G and 6−31G basis sets. The effect of the addn. of polarization functions and the increase of the size of the basis set, in both geometrical and electronic structures, is analyzed in detail. Results are compared to other levels of theory.

C. A. 1996, 124, N 22

Отт. 38500

1996

Si_n
Si_n^-
$(n=2-4)$

Fulara J., Freivogel P.
et al.,

J. Phys. Chem., 1996,
<u>100</u>, 18042 - 18047

$Si_5(2)$ (ОМ. 41795) 1996

Philippe Rocabois,

и.л. Christian Chatillon et al.,

т.ф. High Temperat. — High Pressures, 1995/1996, 27/28, pages 25-39

$Si_6(2)$ Om 41795 1996

Philippe Rocabois,
u·n· Christian Chatillon et al.,
m.p. High Temperat. — High
Pressures, 1995/1996,
27/28, pages 25-39

Si_n

1996

126: 203949j Wave function–based ab initio molecular dynamics of clusters (silicon, lithium). Gibson, Douglas Allen (Univ. of California, Los Angeles, CA USA). **1996.** 166 pp. (Eng). Avail. Univ. Microfilms Int., Order No. DA9704587. From *Diss. Abstr. Int., B* **1997,** 57(9), 5662.

теор. расчет

(Н) Li_n

(см. ориг.)

C. A. 1997, 126, N 15

Si_{60} и др.

1996

/ 125: 42234j **An effective Hamiltonian study for the binding energies of large Si clusters $(Si)_n$.** Oshiro, T.; Lutrus, C. K.; Hagen, D. E.; Lee, Jae Suk; Salk, Sung Ho Suck (Department of Physics, University of Missouri, Rolla, MO 65401 USA). *J. Korean Phys. Soc.* **1996**, 29(2), 200–204 (Eng). In view of the deficiency of information on large Si clusters, a computationally efficient effective Hamiltonian method for Si clusters $(Si)_n$ of large size is employed. The computed results of binding energies for large clusters, including the fullerene (soccer ball) structure of $(Si)_{60}$, are quite encouraging in that the extrapolated value of the av. binding energy from a linear least–squares fit is close to the obsd. bulk value of 4.6 eV. Magic nos. are also found to be close to the obsd. ones. From the present study of predicted magic nos. for $(Si)_n$, we find that the Si clusters do not from tetrahedrally bonded structures even at sufficiently large clusters up to the size of $n = 25$ in $(Si)_n$. It is also shown that the soccer–ball shaped Buckminsterfullerene structure of $(Si)_{60}$ is unstable, indicating that the stable geometric configuration of such a large size cluster is no longer the cage structure seen in small clusters.

теор. расчет энергии связи и структуры

C. A. 1996, 125, N4

Si_n

$n = 11 \div 14$

1996

структура кластеров

125: 177865m Structures of silicon clusters. Pan, Jun; Bahel, Atul; Ramakrishna, Mushti V. (Department Chemistry, New York University, New York, NY 10003-6621 USA). *Surf. Rev. Lett.* **1996**, 3(1), 341–345 (Eng). We detd. the structures of silicon clusters in the 11–14-atom size range using the tight-binding mol. dynamics method. The Si_{11} is an icosahedron with one missing cap, Si_{12} is a complete icosahedron, Si_{13} is a surface-capped icosahedron, and Si_{14} is a 4-4-4 layer structure with two caps. The characteristic feature of these clusters is that they are all surface.

C. A. 1996, 125, N 14

Si_{20}
Si_{21}

1996

126: 162546e Electronic, vibrational and geometrical structure of Si_{20} and Si_{21}. Pederson, M. R.; Jackson, K.; Porezag, D.; Hajnal, Z.; Frauenheim, Th. (Complex Systems Theory Branch, Naval Research Laboratory, Washington, DC 20375–5345 USA). *Int. Conf. Phys. Semicond., 23rd* **1996**, 2, 1657–1660 (Eng). Edited by Scheffler, Matthias; Zimmermann, Roland. World Scientific: Singapore, Singapore. We discuss recent calcns. on new low-energy structures for the Si_{20}– and Si_{21}–clusters. Since it is well known that the no. of metastable geometrical structures grows with the size of the mol. and since it is difficult to directly det. geometries of intermediate-sized clusters from expt., we have developed and applied first-principles methodologies which allow for the calcn. of many phys. observable properties of a given clusters. Calcns. such as the ones presented here should aid in the exptl. identification and characterization of nanoscale silicon clusters.

теорет-
расчет
структур,
Di, стабилн

C. A. 1997, 126, N 12

SiNO
NSiO
SiON

1996

126: 162511q **Isomerism and spin−vibronic energy levels of silicon nitroxide.** Puzzarini, Cristina; Tarroni, Riccardo; Palmieri, Paolo; Carter, Stuart (Dip. Chimica Fisica Inorganica, Univ. Bologna, 40136 Bologna, Italy). *J. Chem. Soc., Faraday Trans.* **1996**, 92(22), 4361−4365 (Eng), Royal Society of Chemistry. The ground−state potential−energy surface of silicon nitroxide has been investigated theor. by the internally contracted multi ref. CI (MRCI) method from complete active space self consistent field (CASSCF) ref. wavefunctions using large orbital expansions. Three different linear isomers have been identified on the ground electronic state potential−energy surface, corresponding to the chem. structures SiNO, NSiO and SiON. Their geometries and relative energies have been estd. Variational theory has been used to calc. the vibronic levels for values of the total angular momentum quantum no. J = 1/2, 3/2, including dynamic non−adiabatic interactions between electronic spin, orbital and vibrational angular momenta. The predicted vibronic frequencies are expected to be accurate for all three isomers.

теор. расч.
стр-ры,
стабилн.

C.A. 1997, 126, N 12

Si$_n$

1996

Zdetsis A. D.,

ab initio
расчет
стабильн.
и
стр-ры

NATO ASI Ser., Ser. B
1996, <u>855</u>, 455-464.

(ал. ● C$_n$; <u>III</u>)

Si_{34}
Si_{46}

1997

128: 107764r **Structural properties and vibrational modes of Si_{34} and Si_{46} clathrates.** Kahn, Daniel; Lu, Jian Ping (Department of Physics and Astronomy, University of North Carolina, Chapel Hill, NC 27599 USA). *Phys. Rev. B: Condens. Matter* 1997, 56(21), 13898−13901 (Eng), American Physical Society. The structural and vibrational properties of the Si clathrates Si_{34} and Si_{46} were studied using the O(N) tight-binding d.−matrix method of Li, Nunes, and Vanderbilt. The elastic moduli are similar to those of cubic−diamond Si. The large unit cells lead to complex Raman and IR spectra which were obtained by calcg. the full dynamical matrix directly. Certain modes are identified as mol.−like. Dispersion relations as well as the vibrational d. of states are computed. The latter shows an unusual gap at ~16.5 THz for both clathrates. The mode−Gruneisen parameters are also calcd.

структура,
ик,
расчет

C.A. 1998, 128, N9

Si_n

1997

127: 40130q **Study on electronic structures of silicon clusters by hetero–atom doping.** Nakajima, Atsushi; Kaya, Koji (Dep. Chem., Fac. Sci. Technol., Keio Univ., Yokohama, Japan 223). *Hyomen Kagaku* 1997, 18(3), 141–148 (Japan), Nippon Hyomen Kagakkai. Electronic properties of small silicon clusters ($n \leq 11$), produced by a laser vaporization method, were investigated by photoelectron spectroscopy of their anions. The doping by F or Na atoms enables us to subtract or add an

(фотоэл-спектр)

C. A. 1997, 127 N3

ОТ 39123 1997

Si_n

n=9-14

стр-ра, спектр, поляр. расч

C.A. 1998, 128, N10

128: 121063t **Structure and vibrational spectra of low-energy silicon clusters.** Sieck, A.; Porezag, D.; Frauenheim, Th.; Pederson, M. R.; Jackson, K. (Institut fur Physik, Technische-Universitat-Chemnitz, D-09107 Chemnitz, Germany). *Phys. Rev. A: At., Mol., Opt. Phys.* **1997**, 56(6), 4890-4898 (Eng), American Physical Society. We have identified low-energy structures of silicon clusters with 9 to 14 atoms using a nonorthogonal tight-binding method (TB) based on d.-functional theory (DF). We have further studied the resulting structures with an accurate all-electron first-principles technique. The results for cohesive energies, cluster geometries, and HOMO-LUMO gaps show an overall good agreement between DF-TB and SCF-DF theory. For Si_9 and Si_{14}, we found equil. structures, whereas for Si_{11}, Si_{12}, and Si_{13}, we present clusters with energies close to that of the corresponding ground-state structure recently proposed in the literature. The bonding scheme of clusters in this size range is different from the bulk tetrahedral symmetry. The most stable structures, characterized by low energies and large HOMO-LUMO gaps, have similar common subunits. To aid in their exptl. identification, we have computed the full vibrational spectra of the structures, along with the Raman activities, IR intensities, and static polarizabilities, using SCF-DF theory within the local-d. approxn. (LDA). This method has already been successfully applied to the detn. of Raman and IR spectra of silicon clusters with 3-8, 10, 13, 20, and 21 atoms.

128: 121064u Simple and

Si_n^- (n=3-7)

От · 39156

1998

Cangshan Xu et al.,

фотоэл. спектр

J. Chem. Phys., 1998, <u>108</u> (4), 1395–

Vibrationally resolved photoelectron spectroscopy of silicon cluster anions Si_n^- $(n=3-7)$.

Si_N (Om- 39780) 1998

Hagelberg F*, et al.,
J. Mol. Struct. (Theochem)
1998, <u>454</u>, 209–216
Theoretical investigations
on small closed-shell
silicon N clusters.

Si_N

1998

N - 4, 6, 7, 10

129: 127419f Global geometry optimization of small silicon clusters at the level of density functional theory. Hartke, Bernd (Institut Theoretische Chemie, Universitaet Stuttgart, D-70569 Stuttgart, Germany). *Theor. Chem. Acc.* **1998**, 99(4), 241–247 (Eng), Springer–Verlag. By application to small Si clusters Si_N (with N = 4,6,7,10) it is shown that truly global geometry optimization on an ab initio or d. functional theory level can be achieved, at a computational cost of approx. 1–5 traditional local optimization runs (depending on cluster size). This extends global optimization from the limited area of empirical potentials into the realm of ab initio quantum chem.

структура, ab initio расчет

CA 1998, 129, №10

Si_n

$n = 9-14$

1998

структурные параметры

129: 207431u First-principles study of the equilibrium structures of Si_n clusters. Jeong, Ji-Wook; Lee, In-Ho; Oh, J. H.; Chang, K. J. (Department of Physics, Korea Advanced Institute of Science and Technology, Taejon, S. Korea). *J. Phys.: Condens. Matter* **1998**, 10(26), 5851–5860 (Eng), Institute of Physics Publishing. We investigate the at. structure of Si_n ($n = 9-14$) clusters using the first-principles pseudopotential method within the local-d.-functional approxn. (LDA). The equil. geometries of small clusters with $n \le 12$ tend to be capped prismatic structures. For $n = 13$, we find a surface-like metallic compact structure which is derived from a capped icosahedron and competes with a stable trigonal prism, while this structure is the most stable for $n = 14$. These results are compatible with the obsd. stability of Si_{13} and Si_{14}, as compared to Si_n clusters with nearby values of n, against chem. reactions with simple mols. The effect of electron-electron correlations on the energetics of isomers with $n = 13$ is examd. through variational quantum Monte Carlo calcns., and the LDA energy ordering remains unchanged, consistently with previous diffusion quantum Monte Carlo calcns.

C. A. 1998, $\underline{129}$, N 16

Si_{13}

1998

129: 193933v **Structures and properties of Si_{13} isomers.** Pan, B. C.; Wang, C. Z.; Turner, D. E.; Ho, K. M. (Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011 USA). *Chem. Phys. Lett.* 1998, 292(1,2), 75–79 (Eng), Elsevier Science B.V.. The structures and properties of several Si_{13} clusters are studied using d. functional calcns. The calcn. results show that a newly discovered structure with C_s symmetry is energetically most favorable. Our calcn. also provides detailed information about the electronic and vibrational properties of the clusters which are useful for understanding the structure and stability of the cluster.

стр-ра √
Di,
стабильн,
расчет

CA-1998, 129, N15

1998

Si_n

$n \le 26$

(D_0)

теор. расчет

130: 71857y **Dissociation Energies of Silicon Clusters: A Depth Gauge for the Global Minimum on the Potential Energy Surface.** Shvartsburg, Alexandre A.; Jarrold, Martin F.; Liu, Bei; Lu, Zhong-Yi; Wang, Cai-Zhuang; Ho, Kai-Ming (Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208 USA). *Phys. Rev. Lett.* 1998, 81(21), 4616–4619 (Eng), American Physical Society. We have modeled the dissocn. of Si_n neutrals and cations in the $n \le 26$ range. The fragmentation pathways up to $n = 26$ and dissocn. energies up to $n = 20$ have been calcd. assuming a statistical decompn. process. The results for the cations are in good agreement with the measurements. This indicates that our search of configuration space for the silicon clusters in this size range has indeed found the global min., viz. a family of "stacked Si_9 tricapped trigonal prisms". This is the first time that dissocn. energies have been used to test the results of a global optimization.

C.A. 1999, 130, N6

F: Si7
P: 3

1999

132:83990 Bonding nature of Si7 bicapped pentagon cluster: ab-initio stud Eguchi, Haruki; Tsumuraya, Kazuo; Nagano, Takatoshi; Kihara, Shigemitsu Research Laboratory, Ishikawajima-Harima Heavy Industries Co., Ltd. Tokyo 135-8732, Japan Mater. Trans., JIM, 40(11), 1198-1204 (English) 1999 The authors studied the bonding in bicapped pentagon Si7 clusters in ter of the Laplacian field of the charge d. The bonding between the capped a the strongest and has a covalent character; the bonding between the edge on the pentagon shows the weakest covalent character. The second deriv. charge d. gives no information on the bonding.

C. A. 2000, 132

Фуллерены 1999

Si_{60} Leszczynski, Jerzy; et al.,

J. Phys. Chem. A 1999,

потенц. ионизации, теорет. расчет

<u>103</u>(3), 396-401

(см. C_{60}, фуллерены; <u>III</u>)

1999

F: Sin
P: 3
131:356319 Ab initio molecular orbital calculations on silica rings. Nede J. M.; Hench, L. L. Department of Materials, Technology and Medicine, Imperial College of Science London, UK J. Non-Cryst. Solids, 255(2,3), 16 170 (English) 1999 The ab initio MO 3-21G method

was applied to silica rings with two to si tetrahedra per ring. The geometries of the rings and their total electro energies are compared with previous ab initio, AM1 and PM3 results and wi exptl. values for amorphous silica. The 3-21G method appears to reproduc accuracy the exptl. results. The semi-empirical PM3 method also gives re that compare favorably with the ab initio calcns. and thus is concluded t suitable for use in calcns. on bigger silica clusters.

Si_n

2001

структура
превращ.,
стабильн.,
процесс
плавления

135: 82218v Structural transition of Si clusters and their thermodynamics. Wang, J.; Wang, G.; Ding, F.; Lee, H.; Shen, W.; Zhao, J. (National Laboratory of Solid State Microstructures, Department of Physics, Nanjing University, Nanjing, Peop. Rep. China 210093). *Chem. Phys. Lett.* 2001, 341(5,6), 529–534 (Eng), Elsevier Science B.V. The lowest energy structures of Si_n clusters up to 21 atoms were optimized with a genetic algorithm (GA) and d. functional theory (DFT) with generalized gradient approxn. (GGA). The structural transition from prolate cage–based structures to near–spherical configurations was found at n=17. Remarkable different melting behaviors of silicon clusters were obtained between those in prolate structures and near–spherical geometries. The structural transformation of near–spherical clusters was obsd. in the melting process. Two possible melting processes are proposed: near–spherical → prolate → subunits → molten and near–spherical → prolate → molten oblate.

C.A. 2001, 135, N6.

Si_6

2001

135: 185751t The real structure of the Si_6 cluster. Zdetsis, Aristides D. (Department of Physics, University of Patras, Patras, Greece GR 26500). *Phys. Rev. A: At., Mol., Opt. Phys.* 2001, 64(2), 023202/1–023202/4 (Eng), American Physical Society. Contrary to well-established recent theor. results based on second-order Moller-Plesset perturbation theory, it is illustrated here that the distorted octahedron of D_{4h} symmetry cannot be the ground state of the "magic" Si_6 cluster, but a transition state, connecting two almost isoenergetic structures of lower symmetry, which can coexist. This conclusion, the consequences of which could be far reaching for other magic clusters, is based on higher-order perturbation theory, accurate coupled-cluster CCSD(T) calcns. and d.-functional theory at the hybrid B3LYP level. The discrepancy is due to the poor convergence of the perturbation expansion, related to the flatness of the energy hypersurface near the min. As a result, the structural and electronic properties of Si_6 are still not well understood, although several suggestions are put forward here.

(стр-ра, теор. расч.)

C.A. 2001, 135, N13

Si_5 От 41400 2002

Si_5^+

Si_5^-

Cunyuan Zhao,

J. Chem. Phys., 2002, 116, N 9, 3690— 3699.

теор. расч.

Geometries and spectroscopic properties of silicon clusters

DM 41400

2002

Si_6
Si_6^+
Si_6^-

Cunyuan Zhao,

J. Chem. Phys., 2002,
116, N 9, 3690-3699

Geometries and spectroscopic
properties of silicon

clusters.

Si_n Оп. 41820 2003.

$(n=11-25)$ Bao-Xing Li, Pei-Lin Cao

стр-ра, et al.,

основн.
состоян. Phys. Lett., 2003, A316,

N 3-4

Ground state stuctures of
Si_n $(n=11-25)$

clusters.