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Optical (Hyper)Polarizabilities of Small Silicon Clusters

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Tapio T. Rantala, Mark I Stockman, Daniel A. Jelski and Thomas F. George

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Departments of Chemistry and Physics
State University of New York at Buffalo
Buffalo, New York 14260

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OPTICAL (HYPER)POLARIZABILITIES OF SMALL SILICON CLUSTERS

TAPIO T. RANTALA[*†], *MARK I. STOCKMAN*[*‡], *DANIEL A. JELSKI*[§] *and THOMAS F. GEORGE*[*]

[*]Departments of Physics & Astronomy and Chemistry, Center for Electronic & Electro-optic Materials, 239 Fronczak Hall, State University of New York at Buffalo, Buffalo, NY 14260

[†]Permanent address: Department of Physics, University of Oulu, SF-90570 Oulu, Finland

[‡]Also with: Institute of Automation & Electrometry, Siberian Branch of the USSR Academy of Sciences, 630090 Novosibirsk, USSR

[§]Department of Chemistry, State University of New York, College at Fredonia, Fredonia, NY 14063

ABSTRACT

Electronic contributions to the optical (hyper)polarizabilities of small silicon clusters are theoretically determined. Geometries and the electronic structures of the clusters are established using the tight-binding model. The nonlinear polarizabilities are found to depend primarily on the symmetry of the cluster and prove to be high for the low-symmetry clusters. Possible experiments and applications are discussed.

INTRODUCTION

Small semiconductor clusters in the range from a few atoms to tens of atoms are of a great interest from the viewpoint of both fundamental science[1–5] and applications.[5–8] Their physical properties (symmetry, electronic structure, optical spectra and transition probabilities) differ significantly from those of the solid state both in the bulk and at the surface, and also from the properties of nanoscale structures, such as quantum dots. Linear and nonlinear optical properties of the latter have been shown to depend strongly on their size in the region of quantum confinement (see, e.g., Refs. 5, 9 and 10). But in these and similar works, the bulk electronic structure of the semiconductor is usually assumed and modelled by free electrons with effective mass. Obviously, this approach is valid only for sufficiently large objects with sizes not less than a few nanometers, containing on the order of 1000 atoms or more.

In the present work, the optical properties of small silicon clusters with 7 – 13 atoms are predicted. For such clusters, the bulk approximation is not valid and the detailed structure becomes important. Much work has been done on the structure of silicon clusters, both experimentally for stability and photofragmentation[1,2] and for optical absorption,[3,4] and theoretically with *ab-initio*-type calculations for smaller[11–13] and other methods for larger[14–19] systems. The approach we use in this paper is based upon the semiempirical tight-binding (TB) model. This model has previously been used[17] to describe the structure of Si_{10} isomers. It is relatively simple, thus allowing the global optimization of the geometry even for comparatively large clusters. Moreover, the TB model couples the geometry to the electronic structure, which we find essential, but which usually is ignored for larger systems.[14,15].

With the TB geometry and electronic structure and using one-electron density matrix techniques, we obtain closed sum-over-one-electron-states expressions from which linear and nonlinear optical polarizabilities of clusters are subsequently computed. These characteristics govern a number of observable effects: light scattering and absorption by clusters, second-harmonic generation (SHG), optical rectification, birefringence induced by optical fields and the Kerr effect, phase conjugation, etc.

THEORY

We write the TB Hamiltonian as[18,20]

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$$H_{TB} = \sum_{\mu a} \varepsilon_a^0 \, a_{\mu a}^\dagger a_{\mu a} + \sum_{\mu a \, \nu b} V_{\mu a \, \nu b} \, a_{\mu a}^\dagger a_{\nu b} \quad . \tag{1}$$

where $a_{\mu a}^\dagger$ and $a_{\mu a}$ are electron creation and annihilation operators in the basis $|\mu a\rangle = \varphi_a(\mathbf{r} - \mathbf{R}_\mu)$, with $\varphi_a = \{3s, 3p_x, 3p_y, 3p_z\}$ as the valence orbitals of silicon atom at the sites μ with coordinates $\mathbf{R}_\mu$. To reproduce the bulk silicon band structure with the nearest-neighbor distance 2.35 Å, the diagonal matrix elements of the Hamiltonian (1) were fitted[20] to the values $\varepsilon_s^0 = -5.25$ eV and $\varepsilon_p^0 = 1.20$ eV, and the off-diagonal elements to $V_{ss\sigma} = -1.938$ eV, $V_{sp\sigma} = 1.745$ eV, $V_{pp\sigma} = 3.050$ eV and $V_{pp\pi} = -1.075$ eV. The off-diagonal matrix elements were taken to behave Slater–Koster–like[21] in their angle and distance dependence, and so their bond length dependence is $1/r^2$ up to 3.3 Å, where we consider the bond to be broken.[17]

The diagonalization of the Hamiltonian gives the one-electron energies ε_p and the eigenvectors $\mathbf{C}_p$. Thus, we can write the one-electron states of the occupied and unoccupied valence levels as

$$|p\rangle = \sum_{\mu a} C_{p\mu a} |\mu a\rangle \quad . \tag{2}$$

and the cohesion energy of the N atoms due to the bond formation, which we call the "band structure" energy, can be written as

$$E_{BS} = \sum_p n_p \varepsilon_p - N \sum_a n_a^0 \varepsilon_a^0 + U \sum_\mu (q_\mu - q_\mu^0)^2 \quad . \tag{3}$$

where n_p and n_a^0 are occupation numbers, and the difference between the two first terms is the stabilization energy of the four free-atom valence levels ε_a^0 due to the bonding. The third term in Eq. (3) is added to include the intra-atomic Coulomb repulsion caused by charge transfer within the cluster, and it is evaluated using the Mulliken charges q_μ and q_μ^0, with the constant U taken to be 1 eV.[18]

A repulsion energy term is finally added to account for the structure of small clusters. It is the sum of interatomic pair potentials $E_d(R_{\mu\nu})$ and a term depending on the bond number N_b,

$$E_R = \sum_{\mu<\nu}^{N} E_d(R_{\mu\nu}) - N \left[c_1 \left(\frac{N_b}{N} \right)^2 + c_2 \left(\frac{N_b}{N} \right) + c_3 \right] \quad . \tag{4}$$

This term has been fitted[18] within the present TB model to reproduce the bulk cohesion energies 4.64 and 4.24 eV for the diamond and FCC structures, respectively, and the *ab initio* potential curve of the silicon dimer. This leads to the constants $c_1 = 0.225$ eV, $c_2 = 1.945$ eV and $c_3 = -1.03$ eV, which therefore set the second term to zero for Si_2. Finally, the total cohesion energy of the cluster is written as a sum of the band structure energy E_{BS} and the repulsion energy E_R,

$$E_{coh} = -(E_{BS} + E_R) \quad , \tag{5}$$

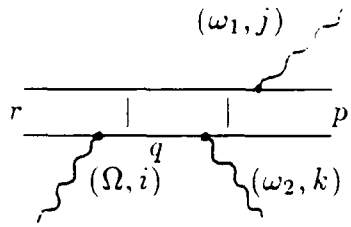
which is maximized to find the structures of the Si clusters in the present work.

The dipole transition matrix elements $(\mathbf{r})_{pq}$ can be written as

$$(\mathbf{r})_{pq} = \sum_{\mu a} C_{q\mu a}^* C_{p\mu a} \mathbf{R}_\mu + \sum_{\mu a b} C_{q\mu b}^* C_{p\mu a} (\mathbf{r})_{ab} \quad , \tag{6}$$

where the atomic transition matrix elements are $(\mathbf{r})_{ab} = \int \varphi_b^*(\mathbf{r}) \, \mathbf{r} \, \varphi_a(\mathbf{r}) \, d\mathbf{r}$.

We use the technique of the one-electron density matrix $\rho_{pq} = \langle a_q^\dagger a_p \rangle$, which exactly takes into account the Fermi statistics of electrons, rather than the conventional many-electron matrix[26,27]. Using this technique, the nth-order polarizability $\alpha^{(n)}$ is conventionally represented by means of double Feynman diagrams. For example, one of the second-order contributions to $\alpha^{(2)}$ is given by



$$= e^2 \sum_{pqr} \frac{(r_k)_{pr}(r_i)_{rq}(r_j)_{qp}}{(-\Omega - \omega_{qr} + i\Gamma_{qr})(\omega_1 - \omega_{pr} + i\Gamma_{pr})} \rho_p^{(0)} \quad . \tag{7}$$

where $\Gamma_{pq} \equiv \Gamma_p + \Gamma_q$ is the pq-transition linewidth. Here one can trace the diagrammatic rules. The horizontal lines correspond to one-electron states over which summation is implied. These lines are separated by vertices, and the vertex between the lower p and q lines corresponds to $-e(\mathbf{r})_{qp}$, and between the upper r and p lines to $e(\mathbf{r})_{pr}$. The vertical line connecting the states r and q denotes the one-electron propagator $[\sum \omega_k - \omega_{qr} + i\Gamma_{qr}]^{-1}$, where $\sum \omega_k$ is the sum of all photon frequencies to the right of the propagator, $\omega_{qr} = (\varepsilon_q - \varepsilon_r)/\hbar$ is the transition frequency between the one-electron states, and the free p lines denote $\rho_p^{(0)}$. The present diagrammatic technique is similar to the conventional one,[26,27] with the difference here that all the operators and states are one-electron ones. The second- and third-order polarizabilities are given by 8 and 48 diagrams, respectively.

NUMERICAL RESULTS

Maximization of E_{coh} (5) yields the cluster structures. The obtained cluster symmetry groups and important electronic structure data are given below in Table 1.

TABLE 1. Structure data for the Si_7, Si_{10} and Si_{13} clusters. The names are from Ref. 17. E_{coh} (eV) is the cohesion energy per atom, and ε_g is the HOMO–LUMO band gap (both in eV and μm).

Name	N	Point group	E_{coh} (eV/atom)	ε_g (eV,	μm)	Coordination min.	max.	av.
	7	D_{5h}	3.8	1.8	0.69	4	6	4.6
DBTA-I	10	C_{2v}	4.0	1.4	0.87	4	7	5.0
TTP	10	C_{3v}	3.9	2.6	0.48	3	6	4.8
TO	10	T_d	3.6	2.9	0.43	3	6	4.8
	13	I_h	4.4	2.8	0.44	6	12	6.7

The linear polarizabilities Re $\alpha_{ij}(\omega)$ (10^{-23} cm^3) of the clusters obtained for different photon energies $\hbar\omega$ are given in Table 2. It follows from this table that Reα is nonsensitive to the symmetry of the cluster, thus bearing little structural information. In contrast, the cluster absorption spectra (See Fig.1), governed by Imα, strongly depend on the cluster structure: the lower the symmetry of the cluster, the richer its spectrum with more red-shifted offset.

The values computed for the second-order polarizabilities (10^{-28} esu) $\beta_{ijk}(\omega, \omega) = \alpha^{(2)}(-2\omega; \omega, \omega)$ and $\beta_{ijk}(-\omega, \omega) = \alpha^{(2)}(0; -\omega, \omega)$, governing SHG and rectification, are given in Table 3 (for the clusters not shown, $\beta = 0$ due to symmetry requirements). It can

TABLE 2

N	Group	ij	$\hbar\omega$ (eV):	0.0	0.5	1.0	1.77	1.5	2.33
7	D_{5h}	xx, yy		8	8	8	9	9	15
		zz		6	6	7	7	7	11
10	C_{2v}	xx		11	12	14	16	38	3
		yy		10	11	11	12	15	8
		zz		14	14	16	18	43	13
10	C_{3v}	xx, yy		12	12	13	13	14	24
		zz		13	13	14	14	15	24
10	T_d	xx, yy, zz		13	13	14	14	15	20
13	I_h	xx, yy, zz		14	14	14	15	15	17

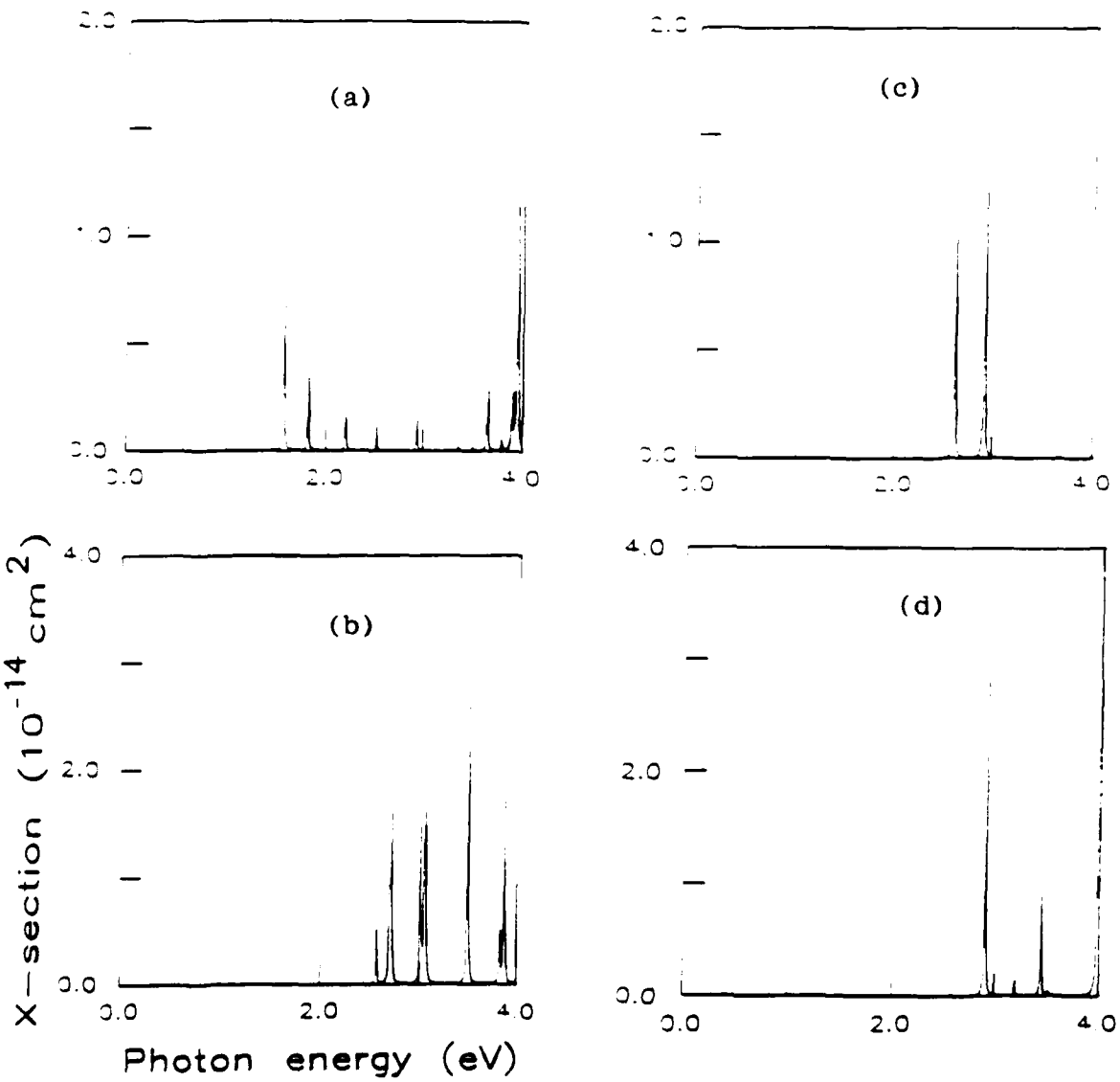


Fig. 1. Absorption spectra of clusters with the names and symmetry groups shown: (a) Si_{10}, DBTA-I (C_{2v}); (b) Si_{10}, TTP (C_{3v}); (c) Si_7, (D_{5h}); (d) Si_{10}, TO (T_d).

TABLE 3

N	ijk	$\hbar\omega$ (eV):	$\alpha^{(2)}(-2\omega;\omega,\omega)$ 0.0	10^{-2}	0.5	1.0	1.17	1.5	$\alpha^{(2)}(0;-\omega,\omega)$ 0.5	1.0	1.17
10 C_{2v}	zzz		-2.9	-2.1	-3.9	5.3	3.9	8.8	-3.6	-8.0	-13.8
	zyy		-1.4	-0.9	-1.6	1.4	-0.3	2.1	-1.7	-3.0	-4.2
	yyz, yzy		-0.9	-0.9	-1.5	8.1	3.5	6.0	-1.1	-2.0	-2.9
	zxx		0.2	0.3	0.8	-3.2	-5.1	-2.4	0.2	-0.0	-0.5
	xxz, xzx		0.4	0.3	0.7	-3.1	6.2	-45.6	0.6	1.6	3.1
10 C_{3v}	zzz		1.8	1.3	1.6	3.7	7.0	31.2	1.9	2.5	2.8
	$yxx, xyx, xxy, -yyy$		0.3	0.3	0.3	0.6	1.0	-4.7	0.3	0.3	0.3
	zxx, zyy		0.8	0.3	0.3	0.4	0.5	-16.0	0.9	1.2	1.4
	xxz, yyz, xzx, yzy		0.2	0.3	0.4	0.9	1.7	16.5	0.2	0.3	0.3
10 T_d	$xyz, xzy,$ $yxz, yzx,$ zxy, xyx		-0.5	-0.2	-0.3	-0.5	-0.8	3.4	-0.5	-0.6	-0.7

be seen from Table 3 that for the lower symmetry clusters C_{2v} and C_{3v} the magnitude of β is considerably higher than for the higher symmetry T_d cluster, reaching values which are characteristic of organic molecules with high nonlinear responses.

The third-order polarizability $\gamma \equiv \alpha^{(3)}$ (data are not shown) is symmetry-allowed in all the cases. Again, the maximum responses are predicted for low-symmetry clusters, reaching high values, $\gamma \approx 2\ 10^{-32}$ esu, for the C_{2v} and C_{3v} clusters.

DISCUSSION

Linear polarizability can be measured for single clusters in experiments using laser light scattering and photon-counting detection. However, this quantity is not sensitive to cluster structure. In contrast, the optical absorption and hyperpolarizabilities do primarily depend upon the cluster symmetry and, therefore, bear important structural information.

The optical absorption of single clusters in jets can be measured similar to Ref. 30 in the following experiment. Clusters are excited by tunable probe radiation and are also subjected to powerful IR radiation which is not absorbed from the ground state but ionizes the clusters already excited by the probe light. The clusters ionized are detected by the mass spectrometer.

The nonlinear optical responses can be detected if it is possible to accumulate clusters in host media. High magnitude of the polarizabilities predicted promises possibility of applications in optical and optoelectronic devices.

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Professor William Unertl
Lab. for Surface Sci. & Technology
University of Maine
Orono, ME 04469

Dr. Terrell Vanderah
Code 3854
Naval Weapons Center
China Lake, CA 93555

Professor John Weaver
Dept. of Chem. & Mat. Sciences
University of Minnesota
Minneapolis, MN 55455

Professor Brad Weiner
Department of Chemistry
University of Puerto Rico
Rio Piedras, Puerto Rico 00931

Professor Robert Whetten
Department of Chemistry
University of California
Los Angeles, CA 90024

Professor R. Stanley Williams
Department of Chemistry
University of California
Los Angeles, CA 90024

Professor Nicholas Winograd
Department of Chemistry
Pennsylvania State University
University Park, PA 16802

Professor Aaron Wold
Department of Chemistry
Brown University
Providence, RI 02912

Professor Vicki Wysocki
Department of Chemistry
Virginia Commonwealth University
Richmond, VA 23284-2006

Professor John Yates
Department of Chemistry
University of Pittsburgh
Pittsburgh, PA 15260