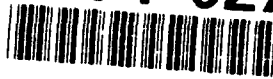


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Ground-state energies of one- and two-electron silicon dots in an amorphous silicon dioxide matrix

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The one- and two-electron ground-state energies of a silicon sphere embedded in an amorphous silicon dioxide matrix are calculated as a function of the sphere size. The electron-electron interaction and polarization effects are treated by perturbation; our quantum-mechanical calculation is valid for small spheres with radii between 10 and 40 Å. For large spheres, classical electrostatics is used. A universal effective capacitance is defined in terms of the difference in the ground-state energies of the $(n + 1)$ - and n -electron cases, which agrees with the usual concept of capacitance in the classical limit.

I. INTRODUCTION

As pointed out by Hayashi,¹ ultrafine particles have properties that suggest many scientific and technological applications. The discovery of luminescence in electrochemically etched silicon is an important scientific breakthrough.² Recently, quantum confinement of microcrystalline silicon (mc-Si) embedded in an amorphous silicon dioxide (a -SiO₂) matrix showed rich structure in tunneling measurements attributable to quantum confinement in three-dimensions.³ Raman scattering from quantum dots of Ge in a -SiO₂ shows the expected downshift from the position of bulk phonons.⁴ Small particles of GaAs (Ref. 5) and CdS (Ref. 6) reveal quantum confinement in optical absorption. The effects of charge accumulation in quantum confinement have been under intensive studies involving quantum dots,⁷ as well as quantum-well structures.^{8,9} It was pointed out that charge accumulation plays a major role in the energy states of the confined mc-Si.³ We are all familiar with the striking difference between the atomic spectra of the hydrogen and helium atoms caused by the presence of additional charge. The physics is even more complicated when the difference in the static dielectric constant of silicon (12) and that of the a -SiO₂ (4) results in induced polarizations. Specifically, a single electron interacts with its induced polarization in the oxide. With two electrons inside the silicon, electrons and induced polarizations interact, resulting in a complicated picture. The present work represents an attempt at understanding the physics involved. Eigenstates of two electrons in such a system can be analytically tractable, provided that spherical geometry is adopted, and may provide insight into the behavior of actual quantum dots. The use of the perturbation theory limits our results essentially to the ground state.

The difference in energy of a two-electron system from a one-electron system may be represented qualitatively by a capacitance. Because of the complicated interactions, this capacitance is not a constant representable only by geometrical considerations. In a large quantum dot approaching the classical limit, the use of a constant capacitance¹⁰ should be a good approximation. It will be made apparent in this work that it is not possible to calculate the effective capacitance of our system in the quantum re-

gime with electrostatics only.

The ground-state energies of a silicon sphere embedded in an amorphous silicon dioxide matrix for one and two electrons are calculated as a function of the size of the sphere. Our results are useful for an understanding of transport measurements, such as resonant tunneling, because the voltages required to bring in additional electrons to the silicon sphere are determined by the ground states. Obviously, excited states must be included in a proper treatment for an understanding of the optical response.

II. MODEL

The model is taken as a silicon sphere of radius a , embedded in an amorphous silicon dioxide matrix. The spherical geometry allows us to make use of the expansion of the Coulomb potential in terms of spherical harmonics, resulting in a separation of the radial and angular components of the wave functions. This, in turn, simplifies the evaluation of various integrals by the orthogonality relationships among the spherical harmonics. The actual barrier height of 3.2 eV between Si and a -SiO₂ is taken to be infinite. This approximation avoids the need to treat the tailing of the wave functions into the a -SiO₂ region for energy calculations, but not for tunneling, of course. The presence of those tails necessitates a replacement of the dielectric discontinuity by a smooth function in order to avoid the singularity of the associated polarization energy.¹¹ Certainly, the approximation of 3.2-eV barrier height by an infinite barrier height should be adequate for most lower states. Obviously this approximation does not apply in the case of GaAs/Al_xGa_{1-x}As dots.

Furthermore, the spherical quantum box must contain enough silicon atoms so that the effective-mass approximation and the static values for permittivity are applicable. These conditions are nearly satisfied for silicon spheres with radius in excess of 10 Å. Because of the presence of the longitudinal and transverse masses, the one-electron states of an isolated silicon sphere require the use of a variational approach¹² which would have been too complicated for us to treat with inclusion of the electron-electron and polarization effects. Therefore, we

have replaced in this work the longitudinal and transverse effective masses by an isotropic mass of $0.26m_e$. The relative permittivities of Si, ϵ_1 , and $a\text{-SiO}_2$, ϵ_2 , are taken to be 12 and 4, respectively.

The Hamiltonian of the system is, as usual, the sum of the kinetic and potential energies. The potential energy is electrostatic in nature, but its form is substantially complicated by the presence of two dielectrics separated by a spherical boundary. We treat this problem by calculating electrostatic-potential-energy terms via the Poisson equation and then using them in the Schrödinger equation.

In a typical resonant-tunneling experiment, the applied voltage measures the energy difference between the ground states of one- and two-electron systems. Our results should therefore be useful in understanding transport measurements. On the other hand, optical measurements involve the occupation of excited states, which is not treated in this work. As mentioned earlier, the major computational difficulties are avoided with the use of an infinite barrier. As long as the excited states for a particular sphere size are much below the 3.2-eV Si/ $a\text{-SiO}_2$ barrier height, excited states may be treated within our present model with only minor additional complexity.

III. ELECTROSTATICS

Calculation of the electrostatic energy terms follows the outlines of the work by Brus and by Böttcher on dielectrics in static electric fields.¹ We cannot apply the image-potential construct, since we deal neither with planar boundaries nor with perfectly conducting spheres. Our chosen approach is to evaluate the electrostatic Green's function for the problem at hand.

The electrostatic potential far away from the sphere is set to zero, leading to the following expressions for the Green's function inside the sphere:

$$G_{\text{in}}(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi\epsilon_0\epsilon_1|\mathbf{r}-\mathbf{r}'|} + \sum_l A_l r^l P_l(\cos\gamma), \quad (3.1)$$

and outside the sphere

$$G_{\text{out}}(\mathbf{r}, \mathbf{r}') = \sum_l B_l r^{-(l+1)} P_l(\cos\gamma), \quad (3.2)$$

in which $\mathbf{r}$ and $\mathbf{r}'$ are the position vectors of the field point and the charge point, respectively, and γ is the angle between these vectors, measured from an origin at the center of the dot.

The coefficients A_l and B_l are determined by the electrostatic boundary conditions at the Si/ $a\text{-SiO}_2$ interface. With the use of an infinite barrier height, the wave functions do not have a tail extending outside of the silicon sphere, so that the coefficients B_l are not needed in the evaluation of matrix elements. Consequently, we only explicitly exhibit the coefficients A_l given by

$$A_l(r') = \frac{(\epsilon_1 - \epsilon_2)(l+1)r'^l}{4\pi\epsilon_0\epsilon_1[\epsilon_2 + l(\epsilon_1 + \epsilon_2)]a^{2l+1}}. \quad (3.3)$$

The form of the electrostatic Green's function allows identification of the potential energy terms in both one-

and two-electron cases. Even in the one-electron case, an electrostatic term arises from the interaction of the electron and bound surface charge density at the spherical boundary of two dielectrics: an electron induces the bound surface charge density which generates electrostatic potential at the electron's position. Energy associated with this term must include a factor of 1/2, since it is a self-interaction term. Therefore, this energy of self-polarization becomes

$$\phi_s(\mathbf{r}) = \frac{1}{2} \sum_l \frac{q^2(\epsilon_1 - \epsilon_2)(l+1)r^{2l}}{4\pi\epsilon_0\epsilon_1[\epsilon_2 + l(\epsilon_1 + \epsilon_2)]a^{2l+1}}, \quad (3.4)$$

where q denotes the electronic charge.

In the two-electron case there are four terms: self-polarization terms for each electron, Coulomb interaction, and polarization interaction. The polarization interaction arises as follows: one electron induces a bound surface charge density which interacts with the second electron. The Coulomb term has the form

$$\phi_C(\mathbf{r}_1, \mathbf{r}_2) = \frac{q^2}{4\pi\epsilon_0\epsilon_1|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (3.5)$$

and from Eqs. (3.1) and (3.3), the polarization term is

$$\phi_p(\mathbf{r}_1, \mathbf{r}_2) = \sum_l \frac{q^2(\epsilon_1 - \epsilon_2)r_1^l r_2^l P_l(\cos\gamma)}{4\pi\epsilon_0\epsilon_1[\epsilon_2 + l(\epsilon_1 + \epsilon_2)]a^{2l+1}}. \quad (3.6)$$

IV. QUANTUM-MECHANICAL CALCULATION

The Hamiltonian for the one-electron case consists of the kinetic energy for the infinite barrier potential, [$V(r)=0$, $r < a$; ∞ , $r > a$] and self-polarization energy. An exact analytical treatment of the Schrödinger equation that uses this Hamiltonian is quite difficult; we therefore resort to the perturbation theory. We can see that for sufficiently small wells, the kinetic energy dominates, and the self-polarization energy can be taken into account by first-order perturbation.

The spherical Bessel functions are the solutions of the zeroth-order Hamiltonian that includes the kinetic energy and infinite barrier potential terms. Dealing with the ground state, we are only interested in the lowest eigenfunction¹⁴

$$\psi_0(\mathbf{r}) = N j_0(\pi r/a) Y_{00}(\Omega), \quad (4.1)$$

where $N = a^{-3/2} I_0^{-1}$ and $I_0^2 = 0.0506606$.

The self-polarization energy term defined by

$$\begin{aligned} E_s &= \langle \psi_0(\mathbf{r}) \phi_s(\mathbf{r}) \psi_0(\mathbf{r}) \rangle \\ &= N^2 \int j_0^2(\pi r/a) Y_{00}^2(\Omega) \\ &\quad \times \left[\sum_l \frac{q^2(\epsilon_1 - \epsilon_2)(l+1)r^{2l}}{8\pi\epsilon_0\epsilon_1[\epsilon_2 + l(\epsilon_1 + \epsilon_2)]a^{2l+1}} \right] r^2 dr d\Omega \end{aligned} \quad (4.2a)$$

contains a dimensionless series,

$$\sum_l \frac{l+1}{\epsilon_1 + l(\epsilon_1 + \epsilon_2)} \int_0^1 x^{2l} j_0^2(\pi x) x^2 dx, \quad (4.2b)$$

which is summed numerically and is equal to 0.015 16. The final form of the self-polarization energy for the ground state is thus

$$E_s = \frac{q^2(\epsilon_1 - \epsilon_2)}{8\pi\epsilon_0\epsilon_1 a} 0.299. \quad (4.3)$$

Note that the self-polarization energy scales as the inverse of the radius and is proportional to the difference of the dielectric constants of the two media.

The total ground-state energy of our model system is represented by the following expression:

$$E_1 = 144.6/a^2 + 1.44/a, \quad (4.4)$$

where the energy is given in eV and the radius a in angstroms.

Table I shows ground-state energies for several sphere radii. Subscripts 1 and 2 of energy E denote number of electrons in the system. The meaning of the superscripts is the following: k for kinetic energy, s for self-polarization, C and p for Coulomb and polarization interactions, respectively, of two electrons, and no superscript for total ground-state energy. The two-electron entries into the table will be described and evaluated immediately. The last row of the table, marked Δ , shows the difference in the ground-state energies between two- and one-electron systems.

The two-electron Hamiltonian includes one-electron terms as before and the Coulomb and polarization terms of the two-electron interaction

$$H = \frac{-\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) + V(r_1) + V(r_2) + \phi_s(r_1) + \phi_s(r_2) + \phi_C(r_1, r_2) + \phi_p(r_1, r_2). \quad (4.5)$$

Once again, we choose to treat the kinetic energy for the infinite barrier as the zeroth order. The other terms are treated by first-order perturbation theory. The lowest-order spherical Bessel function is taken as the spatial wave function for each electron in the ground state. Antisymmetrization is achieved through spin components.

The one-electron terms of the two-electron ground-state energy are the same as in the one-electron case discussed earlier. We need to evaluate only Coulomb and polarization matrix elements. Evaluation of the Coulomb matrix element proceeds in a manner similar to the perturbation treatment of the helium ground state.^{14,15} Its form is

$$E_c = \left\langle \psi_0(r_1) \psi_0(r_2) \frac{q^2}{4\pi\epsilon_0\epsilon_1 |r_1 - r_2|} \psi_0(r_1) \psi_0(r_2) \right\rangle, \quad (4.6)$$

which is reducible to the following:

$$E_c = \frac{q^2}{4\pi\epsilon_0\epsilon_1 a} I_0^{-4} \int_0^1 \int_0^1 j_0^2(\pi x_1) j_0^2(\pi x_2) \times \frac{1}{x_1 x_2} dx_1 dx_2. \quad (4.7)$$

The dimensionless double integral is calculated numerically and its value is 0.004 585 45. The polarization matrix element

$$E_p = \left\langle \psi_0(r_1) \psi_0(r_2) \left[\sum_l \frac{q^2(\epsilon_1 - \epsilon_2)(l+1)r_1^l r_2^l P_l(\cos\gamma)}{4\pi\epsilon_0\epsilon_1 [\epsilon_2 + l(\epsilon_1 + \epsilon_2)] a^{2l+1}} \right] \times \psi_0(r_1) \psi_0(r_2) \right\rangle \quad (4.8)$$

is substantially simplified after the application of the orthogonality relations for the spherical harmonics, because all terms except $l=0$ vanish. The final value of the polarization energy is

$$E_p = \frac{q^2(\epsilon_1 - \epsilon_2)}{4\pi\epsilon_0\epsilon_1 \epsilon_2 a}. \quad (4.9)$$

We stress that self-polarization energy contains contributions from all Legendre polynomials, while both Coulomb and polarization energies contain only the $l=0$ term.

The two-electron ground-state energy can be written as

$$E_2 = 289.3/a^2 + 7.42/a. \quad (4.10)$$

The kinetic-energy term becomes equal to the other components of the total energy at the radius of 39 Å, therefore we do not list E_2 in Table I beyond 40 Å. For a larger radius, a self-consistent calculation cannot be avoided. The two-electron ground-state energy and its various components are included in Table I together with one-electron energy. The difference between two-electron and one-electron ground-state energies is also shown.

V. CLASSICAL CALCULATION

The behavior of the system for a very large spherical well approaches its classical limit. The length scale is set up by an electron coherence length that is taken to be 100 Å. For spherical wells with radii of 100 Å and larger, the

TABLE I. Calculated one- and two-electron ground-state energies from quantum mechanics.

a (Å)	10	20	30	40	60	80
E_1^k (eV)	1.446	0.362	0.161	0.091	0.040	0.023
E_1^s (eV)	0.144	0.072	0.048	0.036	0.024	0.016
E_1 (eV)	1.59	0.434	0.209	0.121	0.064	0.039
E_2^k (eV)	2.893	0.723	0.321	0.182		
E_2^s (eV)	0.288	0.144	0.096	0.072		
E_2^C (eV)	0.214	0.107	0.071	0.054		
E_2^p (eV)	0.24	0.12	0.08	0.06		
E_2 (eV)	3.635	1.094	0.568	0.368		
Δ (eV)	2.05	0.66	0.36	0.25		

electron kinetic energy is estimated via the uncertainty principle. The estimate is of the order of 1 meV, which is negligible compared with the electrostatic contribution. Evaluation of the electrostatic energy requires that one specifies electronic positions. A single electron in the system has its polarization energy minimum at the center of the well. The easiest way to calculate the energy in this case is via energy density. The expression that needs to be evaluated is

$$E_1^C = \frac{1}{2} \left[\frac{1}{\epsilon_2} - \frac{1}{\epsilon_1} \right] \int_a^\infty \frac{D^2}{\epsilon_0} d^3r$$

$$= \frac{1}{2} \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 \epsilon_2} \int_a^\infty 4\pi q^2 \frac{r^2}{16\pi^2 \epsilon_0 r^4} dr, \quad (5.1)$$

leading to the following:

$$E_1^C = \frac{1}{2} \left[\frac{\epsilon_1}{\epsilon_2} - 1 \right] \frac{q^2}{4\pi\epsilon_0\epsilon_1 a}. \quad (5.2)$$

In order to find the positions of the two electrons, the classical ground-state energy in the two-electron case is determined by the minimum of the competing repulsive components. Coulomb and polarization interactions push the electrons apart, towards the well's boundary, while the self-polarization terms push the electrons away from the boundary, closer to each other. The electrons are located at the same distance from the spherical-well's center opposite to each other. The distance from the center, denoted by b , is obtained by minimization of the total electrostatic energy

$$E_2^C \frac{q^2}{4\pi\epsilon_0\epsilon_1} \left[\frac{1}{2b} + \sum_l \frac{(\epsilon_1 - \epsilon_2)b^{2l}(l+1)(-1)^l}{a^{2l+1}[\epsilon_2 + l(\epsilon_1 + \epsilon_2)]} \right. \\ \left. + \sum_l \frac{(\epsilon_1 - \epsilon_2)b^{2l}(l+1)}{a^{2l+1}[\epsilon_2 + l(\epsilon_1 + \epsilon_2)]} \right]. \quad (5.3)$$

The above expression can be written as a function of the ratio between an electron's distance from the center and the well's radius, $x = b/a$:

$$E_2^C = \frac{q^2}{4\pi\epsilon_0\epsilon_1 a} \left[\frac{1}{2x} + (\epsilon_1 - \epsilon_2) \sum_l \frac{x^{2l}(l+1)[1 + (-1)^l]}{\epsilon_2 + l(\epsilon_1 + \epsilon_2)} \right]. \quad (5.4)$$

The minimum with respect to x is found numerically. Its value is 5.0284 at $x = 0.594$.

Table II shows values of the one- and two-electron ground-state energies and their difference computed classically for several radii of the spherical well. The meaning of the symbols is the same as in Table I. We include the radii smaller than 100 Å to emphasize the difference

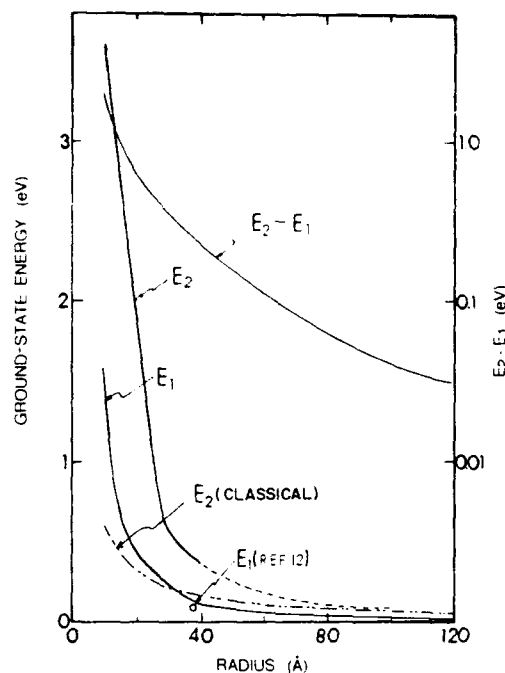


FIG. 1. Ground-state energy of one- and two-electron systems with respect to the spherical-well radius. The dashed portion of E_2 represents an extrapolation to agree with the classical calculation for large a .

between the electrostatic energy computed classically and quantum mechanically. The electrostatic energy computed classically is a mathematically well-defined quantity for radii less than 100 Å, although it loses physical meaning in this range. We plot the ground-state energy of one- and two-electron systems with respect to the spherical-well radius in Fig. 1. Since we restrict a to 39 Å or less, E_2 for a greater than 30 Å is obtained by a smooth-curve fit through E_2 at 39 and 120 Å obtained classically.

VI. DISCUSSION AND CONCLUSIONS

In this work an attempt to model three-dimensional quantum confinement in Si nanometer-sized crystals surrounded by an a -SiO₂ matrix is presented. We are interested in the applied voltage required for tunneling of initially one and then two electrons through the quantum well. A single electron tunnels when the applied voltage aligns the Fermi level of the outside (degenerate) electron reservoir with the one-electron ground-state energy of the well. Additional voltage is necessary to have two electrons tunnel through the well. This voltage is equal to

TABLE II. Classically calculated one- and two-electron electrostatic energies.

a (Å)	10	20	30	40	60	80	100	120
E_1^C (eV)	0.12	0.06	0.04	0.03	0.02	0.015	0.012	0.01
E_2^C (eV)	0.60	0.30	0.20	0.15	0.10	0.075	0.06	0.05
Δ (eV)	0.48	0.24	0.16	0.12	0.08	0.06	0.048	0.04

the difference of the ground-state energies between two- and one-electron systems.

Our model is a compromise between computational feasibility and the need to include all physically relevant terms in the energy. We evaluate the energy in two computationally convenient limits: for very small wells in which the kinetic energy dominates, so that polarization energy may be treated as a perturbation; and for wells large enough so that the situation can be considered classically. Our intuition led us to view the problem of two electrons in a small well as a cross between the helium-atom and particle-in-a-box problems. The helium-atom model supports the suitability of the perturbation theory to deal with electron interactions in the ground state. The particle-in-a-box approach permits the use of the infinite-barrier potential, thus allowing vanishing boundary conditions for the electron wave function at the dielectric boundary to be set up.

In the classical limit, in order to apply electrostatics, we need to specify the positions of the two electrons; therefore, a minimization of the total electrostatic energy is necessary. The two electrons are located at $(r=b, \theta=0)$ and $(r=b, \theta=\pi)$. Consequently, the quantum-mechanical wave functions for the two electrons cannot be represented by the zeroth-order spherical Bessel function, even for small well sizes. This fact clearly points out the limitation in the applicability of the present perturbation calculation.

It is important to note that all the electrostatic terms present have been fully taken into account. Our results clearly indicate the importance of the self-polarization and polarization interaction terms, which have comparable magnitudes but apparently are somewhat larger than the Coulomb interaction. Therefore, the use of a voltage-independent capacitance^{3,10} to deal with the effects of charge accumulation does not offer a clear physical insight. The most physically correct definition of the capacitance should correspond to what may be measured. Consequently, we define an effective capacitance C_{eff} in terms of an increment of the total stored energy in the system. For the particular case of one- and two-electron systems, C_{eff} may be defined by

$$E_2 - E_1 = \frac{1}{2} \frac{q^2}{C_{\text{eff}}} \quad (6.1)$$

This universal definition of C_{eff} gives values for smaller spheres far below what can be calculated from classical

electrostatics. Since we assume C_{eff} at 120 Å is adequately represented by its classical value, at 60 and 30 Å, C_{eff} is only one-half and one-third as large as the classical values, respectively. It is important to note that the usual concept of a capacitance is meaningful in the classical limit.

Our calculations on a suitably defined model system cover the ground-state energies of relatively small and relatively large quantum wells. We believe that ground-state energies of the intermediate quantum wells can be obtained to a fair degree of accuracy by a smooth interpolation scheme. We also believe that we have set the correct voltage scale as high as 1 V for the problem we dealt with, which is much larger than the corresponding scale for GaAs.

Extension of our results to a larger number of electrons and excited states faces severe calculational impediments. The infinite-barrier approximation is less valid in the case of a larger number of electrons than it is for the excited states of one- and two-electron systems. The utilization of a finite barrier immediately introduces a gamut of difficulties: electron wave functions extend a tail across the dielectric boundary, which prohibits the use of the dielectric-constant discontinuity at the boundary, leading to a complicated electrostatic problem. The difficulties are compounded by the need to mix in higher spherical Bessel functions and spherical harmonics to describe correctly the situation in the well. Everything points to a difficult problem that cannot be dealt with analytically but only numerically. Our work has elucidated the major physics of the problem without sacrificing too much rigor, while maintaining computational simplicity and feasibility. As pointed out previously, the problem involving low-lying excited states should be tractable for one- and two-electron systems, with use of the infinite barrier. Therefore, optical transitions between the ground state and the first excited state should not be too much more complicated, when treated within the framework of our model.

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