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Effect of dielectric screening on the donor binding energy in silicon and germanium

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The linear Thomas-Fermi dielectric screening and its various improvements are used to calculate the donor binding energy in silicon and germanium. The results are compared with experimental values.

The binding energies as calculated from the effective-mass theory of shallow impurities are known to agree well with experiment in the case of impurity excited states. However, for the impurity ground states, there is a serious disagreement between theory and experiment.[1-3] In the calculation of the ground states of shallow impurities in semiconductors, the accurate inclusion of the dielectric screening is essential. In the present paper we investigate the effect of the Thomas-Fermi (TF) dielectric screening as proposed by Resta,[4] and its various improvements, on the ground-state binding energy of impurities in silicon and germanium.

Resta[4] has developed a TF theory of dielectric screening in semiconductors. He has used atomic units: $e^2=1$, $\hbar=1$, $m_e=1$, and unless specified otherwise, we shall do the same in the present paper. In Resta's theory, the displaced charge density in a semiconductor has a finite radius R, and the equations to be solved for the self-consistent screened potential $V(r)$ are

$$\nabla^2 V(r)=\begin{cases}(2^{7/2}/3\pi)\{E_F^{3/2}-[E_F+V(R)-V(r)]^{3/2}\}\ , & r\le R \quad (1)\\ 0,\quad r\ge R\ , & (2)\end{cases}$$

where E_F is the valence Fermi energy.

Equation (1) was linearized to

$$\nabla^2 V(r)=q^2[V(r)-V(R)]\ , \tag{3}$$

where $q=(4k_F/\pi)^{1/2}$, with $k_F^2=2E_F$.

For $r\ge R$, Eq. (2) is readily solved to give

$$V(r)=-Z/\epsilon(0)r\ , \tag{4}$$

where $\epsilon(0)$ is the static dielectric constant.

Inside the screening radius R, Resta obtains the following expression for the potential from Eq. (3):

$$V(r)=-\frac{Z}{r}\frac{\sinh[q(R-r)]}{\sinh(qR)}-\frac{Z}{\epsilon(0)R}\ . \tag{5}$$

The screening radius R is found by imposing continuity of electric field at $r=R$. Thus

$$\sinh(qR)/qR=\epsilon(0)\ . \tag{6}$$

The spatial dielectric function $\bar{\epsilon}(r)$ is defined by

$$V(r)=-Z/r\bar{\epsilon}(r)\ . \tag{7}$$

Thus from (4) and (5), using (6), Resta gets

$$\bar{\epsilon}(r)=\begin{cases}\epsilon(0)qR/[\sinh q(R-r)+qr], & r\le R \quad (8a)\\ \epsilon(0),\quad r\ge R\ . & (8b)\end{cases}$$

The values of q and R for silicon and germanium, as obtained in Ref. 4 and corrected in Ref. 5, are shown in Table I against "Linear TF." For the effective mass, we quote here some of the values which have been used by different workers. (a) Silicon: $m^*/m_e=0.306$ (Csavinszky[6]), 0.31 (Breitenecker, Sexl, and Thirring[7]), 0.293 (Müller[8]), 0.292 (Morita and Nara[9]), 0.298 19 (Ning and Sah[10]), 0.31 (Jaros[11]), 0.2987 (Resca and Resta[12]). We adopt here $m^*/m_e=0.30$. (b) Germanium: $m^*/m_e=0.173$ (Csavinszky[6]), 0.18 (Breitenecker, Sexl, and Thirring[7]), 0.17 (Jaros[11]). We adopt here $m^*/m_e=0.17$ for germanium. Following Resta and several other papers in this field, $\epsilon(0)$ was taken to be 11.94 for silicon and 16.0 for germanium, though these are not the best values. The ground-state binding energy was calculated from the potential (7) by numerical integration of the Schrödinger equation using Numerov's method and a logarithmic mesh and the results are shown in Table II.

Cornolti and Resta[5] have obtained the numerical solution of the nonlinear TF equation (1) and have given

TABLE I. The parameters q and R of Eq. (8). The values with asterisks were obtained in this paper, see text.

	Silicon		Germanium		
	q	R	q	R	Source
Linear TF	1.10	4.28	1.12	4.54	Refs. 4 and 5
Nonlinear TF	1.12*	4.06	1.135*	4.33	Ref. 5
Linear TFD	1.35	3.50	1.36	3.74	Ref. 16
Nonlinear TFD	1.344*	3.34	1.354*	3.60	Ref. 16

TABLE II. Ground-state binding energy for a donor impurity in silicon and germanium.

Method	Silicon (meV)	Germanium (meV)
Hydrogenic	28.6	9.0
Linear TF	128	50
Nonlinear TF	69	22
Linear TFD	62	19
Nonlinear TFD	43	13
Experimental (Refs. 17–19)	45.5 (P)	12.9 (P)
	53.7 (As)	14.17 (As)
	42.7 (Sb)	10.32 (Sb)

figures showing $\bar{\epsilon}(r)$ as a function of r for diamond, Si, and Ge for $Z=\pm1,\pm4$. In the calculation of the binding energy, it is convenient if the potential is available in an analytical form. The shapes of $\bar{\epsilon}(r)$ curves for the linear TF and nonlinear TF cases are very similar. It was found that for the nonlinear TF case, the curves given by Cornolti and Resta[5] can also be represented by Eq. (8a) provided q and R are suitably chosen. R was given the same value as obtained by Cornolti and Resta and q was obtained empirically. This procedure, however, leads to a discontinuity in the electric field at $r=R$. For the purpose of obtaining the binding energy, this is, however, not important. The values of q thus obtained are shown in Table I against "Nonlinear TF" and the corresponding binding energies are shown in Table II. Csavinszky and Brownstein[13] and Chao[14] have obtained approximate solutions of the nonlinear TF equation of Resta.

The TF theory for free atoms and ions was improved by Dirac by the inclusion of exchange. The improved version is known as the Thomas-Fermi-Dirac (TFD) theory. Csavinszky[15] and Scarfone[16] have extended the linear TF theory for impurities in semiconductors to include exchange. The solution of the resulting equation gives $\bar{\epsilon}(r)$ of the same analytical form as Eq. (8), but the expression for q is different from the linear TF case. We may also note here that the expressions for q as given by Csavinszky[15] and Scarfone[16] are different and lead to very different numerical q values. In the present paper we shall use Scarfone's values, which are given in Table I, and the corresponding calculated binding energies are recorded in Table II.

Scarfone[16] has also solved the nonlinear TFD screening equation for impurities by numerical methods for diamond, silicon, and germanium. He presents his results in the form of $\bar{\epsilon}(r)$ versus r curves for $Z=\pm1$, ±2, ±3, and ±4. Here also it was found that for $Z=1$, the given curves can be represented by Eq. (8a) by empirically chosen values of q, and R having the same value as calculated by Scarfone. These values of q and R are shown in Table I and the corresponding binding energies in Table II. The experimental values[17–19] of ground-state binding energies for P, As, and Sb are also shown in Table II.

We next consider the results. The linear TF binding-energy values are seen to be very large as compared to the experimental ones. The range of validity of the linearized theory has been investigated by Csavinszky.[20] He finds that for $Z=1$ the linearized TF equation is not valid for a space region of about $\frac{1}{5}$ of the screening radius. Our results clearly indicate that the linear TF approximation is highly inadequate.

The results from the "nonlinear TF" and "linear TFD" dielectric screening are not too different. It would appear that nonlinearity effects and exchange are about equally important.

Our results clearly show that the ground-state binding energy is very sensitive to the form of the dielectric screening. The best results are obtained from the nonlinear TFD dielectric screening. Both for silicon and germanium the calculated binding energy is quite close to the experimental values. The results appear to indicate that the influence of the chemical identity of the donor is small for P and Sb in the case of silicon, and that of P and As in the case of germanium.

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