Ab initio calculation of the macroscopic dielectric constant in silicon

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We perform a first-principles calculation of the static dielectric constant of Si in the framework of density-functional theory. The only essential approximation used in this work is the local-density approximation (LDA): norm-conserving pseudopotentials and large plane-wave basis sets are used, numerical roundoff and convergence errors are kept below 1%. The present calculation gives for the first time the "exact" value of the macroscopic dielectric constant at the LDA level. The theoretical value of ϵ_∞ is 12% higher than experiment.

I. INTRODUCTION

In recent years a considerable amount of experience has been gained in the first-principle calculation of ground-state properties of the simplest semiconductors within the framework of the density-functional theory (DFT).[1-3] The state-of-the-art accuracy of the current calculations is such that the only essential approximation made is the use of the local-density approximation (LDA).[4]

A striking agreement between first-principle calculations and experimental data has been found for a number of physical properties: the theory predicts the observed crystal structures, lattice constants, elastic constants, and phonon frequencies within a few percent from the experiment.[4,5] This is indeed much better than expected, before the starting of the present day intensive computational investigations; some reasons have been put forward to explain why LDA works so well beyond the limits of applicability originally proposed for it.[6] Because of such a successful experience, LDA has become the reference tool to deal with the electronic ground state of real semiconductors. The application of LDA to properties other than those traditionally dealt within this approximation constitutes not only an interesting extension of the present first-principle investigation of real solids, but also provides valuable information to assess the limitations intrinsic to the LDA itself.

In this paper, the macroscopic dielectric constant of Si is calculated for the first time from first principles, within the LDA, using all the state-of-the-art ingredients for the theoretical description of electronic ground states, namely norm-conserving pseudopotentials and large plane-wave basis sets. The linear response within the DFT is exactly expressed through a straightforward modification of the random-phase approximation (RPA).[7] Local-field effects are accounted for, as usual, through the inversion of large dielectric matrices.[8,9] Although the present formulation is RPA based and involves, as such, perturbation sums over the crystal conduction states, we stress that the static dielectric constant we are calculating is a property of the electronic ground state, to which DFT strictly applies. In fact, the static dielectric response can be generally obtained from the functional derivative of the electron density with respect to the external potential. The basic question we address here is to which accuracy LDA is able to predict the static electronic dielectric constant of covalent semiconductors. Previous calculations within the LDA were performed using local pseudopotentials; they were affected by convergence problems, and do not agree in the value of the calculated dielectric constant.[10-12] In this work a final issue to this question is given.

II. BASIC THEORY

Within the DFT, one can define the independent-electron polarizability χ_0 as the functional derivative of the electron density with respect to the total Kohn-Sham potential,[13] evaluated at the unperturbed electronic ground state. In a periodic medium, χ_0 is, at any given $\mathbf{q}$ point in the Brillouin zone (BZ), a matrix over reciprocal-lattice vectors whose expression was first given by Adler and Wiser[7] in the context of the self-consistent field (SCF) approximation

$$\chi_0(\mathbf{q}+\mathbf{G},\mathbf{q}+\mathbf{G}')=-\frac{4}{(2\pi)^3}\sum_{v,c}\int_{\mathrm{BZ}}d\mathbf{k}\frac{\langle\mathbf{k}+\mathbf{q},c\,|\,e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}\,|\,\mathbf{k},v\rangle\langle\mathbf{k},v\,|\,e^{-i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}}\,|\,\mathbf{k}+\mathbf{q},c\rangle}{E_c(\mathbf{k}+\mathbf{q})-E_v(\mathbf{k})}\,, \tag{1}$$

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where $E_b(\mathbf{k})$ and $|\mathbf{k},b\rangle$ are, respectively, eigenvalues and eigenfunctions of the Kohn-Sham unperturbed crystal Hamiltonian. (Atomic units are used throughout.)

If exchange and correlation (xc) effects on the response are neglected, χ_0 directly yields the usual RPA expression for the dielectric matrix:

$$\epsilon_{\mathrm{RPA}}(\mathbf{q}+\mathbf{G},\mathbf{q}+\mathbf{G}') = \delta_{\mathbf{G},\mathbf{G}'} - 4\pi\chi_0(\mathbf{q}+\mathbf{G},\mathbf{q}+\mathbf{G}')/|\mathbf{q}+\mathbf{G}|^2 \quad (2)$$

or, in shorthand,

$$\epsilon_{\mathrm{RPA}} = 1 - v_c\chi_0 \,. \quad (3)$$

In the following, expressions (2) and (3) are calculated from the LDA band structure and will be simply referred to as RPA dielectric matrices. Within the DFT, it can easily be proved[10,13] that the exact expression for the dielectric matrix is

$$\epsilon_{\mathrm{LDA}} = 1 - v_c\chi_0(1 - f_{\mathrm{xc}}\chi_0)^{-1}, \quad (4)$$

where f_{xc} is the functional derivative of the xc potential with respect to the electron density

$$f_{\mathrm{xc}}(1,2) = \delta V_{\mathrm{xc}}(1)/\delta n(2) \quad (5)$$

evaluated at the unperturbed ground state. The exact form of the operator f_{xc} is of course unknown, and Eq. (4) is useless unless some approximate form of it can be used. In the LDA, f_{xc} turns out to be a local operator in $\mathbf{r}$ space, which can be easily evaluated in reciprocal space using fast-Fourier-transform techniques. Use of such a f_{xc} in Eq. (4) together with χ_0 calculated from LDA energy bands, gives us a dielectric matrix which is the exact response function at the LDA level.

The macroscopic dielectric constant ϵ_∞ is the inverse of the long-wavelength ($\mathbf{q}\to 0$) limit of the $\mathbf{G}=\mathbf{G}'=0$ element of the inverse dielectric matrix (IDM):

$$\epsilon_\infty = 1/\epsilon^{-1}(0,0) \equiv 1/\lim_{\mathbf{q}\to 0}[\epsilon^{-1}(\mathbf{q},\mathbf{q})] \,. \quad (6)$$

In a cubic material, the $\mathbf{q}\to 0$ limit of the $\mathbf{G}=\mathbf{G}'=0$ matrix element of any totally symmetric operator is analytic. Therefore we use, in Eq. (6), as well as in the following, the shorthand notation (0,0) to indicate unambiguously such $\mathbf{q}\to 0$ limit. The IDM has nonvanishing off-diagonal elements—due to lattice periodicity—which generate "umklapp" effects in the response. These are generally referred to as "local-field effects". As far as ϵ_∞ is concerned, the basic local-field effect is that this is different (smaller, as we will see) from just the (0,0) element of the direct dielectric matrix.

Up to now we have summarized rather well-known general results. In the remainder of this section we focus on three important points which are relevant to the present work, and which are often overlooked in the literature, namely: the sign of both local-field and exchange-correlation effects on the macroscopic dielectric constant of a crystal, and the evaluation of long-wavelength limits in the presence of nonlocal pseudopotentials.

In order to discuss the above corrections, it is convenient to perform a simple transformation on ϵ and deal with Hermitian dielectric matrices. To this aim we define the "Hermitian dielectric matrix" as

$$\tilde{\epsilon} = v_c^{-1/2}\epsilon v_c^{1/2} \,. \quad (7)$$

We notice in particular that $\tilde{\epsilon}(0,0)=\epsilon(0,0)$ and $\tilde{\epsilon}^{-1}(0,0)=\epsilon^{-1}(0,0)$.

We first discuss the sign of the xc correction to the RPA results. In terms of $\tilde{\epsilon}$, Eq. (4) reads as

$$\tilde{\epsilon}_{\mathrm{LDA}} = 1 - v_c^{1/2}\chi_0(1 - f_{\mathrm{xc}}\chi_0)^{-1}v_c^{1/2} \,. \quad (8)$$

An expansion of Eq. (8) in powers of f_{xc} shows that

$$\tilde{\epsilon}_{\mathrm{LDA}} = \tilde{\epsilon}_{\mathrm{RPA}} - v_c^{1/2}\chi_0 f_{\mathrm{xc}}\chi_0 v_c^{1/2} - v_c^{1/2}\chi_0 f_{\mathrm{xc}}\chi_0 f_{\mathrm{xc}}\chi_0 v_c^{1/2} - \cdots \,. \quad (9)$$

It is easy to realize that, within the LDA, the operator f_{xc} is negative definite since the xc potential is a negative function monotonically decreasing with increasing density. Since both f_{xc} and χ_0 (Ref. 14) are negative definite, one has that $\tilde{\epsilon}_{\mathrm{LDA}} - \tilde{\epsilon}_{\mathrm{RPA}}$ is positive definite. A similar argument also proves that $\tilde{\epsilon}^{-1}_{\mathrm{LDA}} - \tilde{\epsilon}^{-1}_{\mathrm{RPA}}$ is negative definite. Therefore, $\epsilon_{\infty\,\mathrm{LDA}} > \epsilon_{\infty\,\mathrm{RPA}}$.

The second point concerns the sign of local-field effects on ϵ_∞. All previous calculations, as well as our results, indicate that

$$\epsilon_\infty = 1/\epsilon^{-1}(0,0) < \epsilon(0,0) \,. \quad (10)$$

This relationship for the static response matrices follows from the requirements of stability of the system and of causality. Let us block partition the matrix $\tilde{\epsilon}$ in the $\mathbf{q}\to 0$ limit as

$$\tilde{\epsilon} = \begin{bmatrix} \epsilon(0,0) & W^\dagger \\ W & B \end{bmatrix}, \quad (11)$$

where the "body" B is obtained from $\tilde{\epsilon}$ just suppressing the first row ($\mathbf{G}=0$) and the first column ($\mathbf{G}'=0$). It has been shown[14,15] that, due to stability and causality requirements, both $\tilde{\epsilon}$ and B are positive definite within RPA. Now performing a block inversion of Eq. (11) we obtain

$$\tilde{\epsilon}^{-1}(0,0) = 1/[\epsilon(0,0) - W^\dagger B^{-1} W], \quad (12)$$

which proves Eq. (10) at the RPA level.

Going beyond RPA and considering xc effects, the above requirements only impose that $B^{-1}-1$ is negative definite, which is consistent, at least in principle, with negative eigenvalues of B^{-1}. However, in all those cases where the xc effects are not too large and the approximate expansion given in Eq. (9) holds, the conclusions drawn within RPA maintain their validity within LDA.

The third point concerns the evaluation of long-wavelength limits in the presence of nonlocal pseudopotentials. In Eq. (1), the typical matrix element one has to calculate for $\mathbf{G}=0$ or $\mathbf{G}'=0$ is

$$\langle \mathbf{k}+\mathbf{q},c \,|\, e^{i\mathbf{q}\cdot\mathbf{r}} \,|\, \mathbf{k},v\rangle \simeq i\mathbf{q}\cdot\langle \mathbf{k},c \,|\, \mathbf{r} \,|\, \mathbf{k},v\rangle \,. \quad (13)$$

The matrix elements of $\mathbf{r}$ are ill defined when wave functions obey Born—von Kármán boundary conditions: As a consequence, one is forced to evaluate them (when possible) using the commutator of $\mathbf{r}$ and the crystal self-

consistent field Hamiltonian $H_{\rm SCF}$:

$$\langle \mathbf{k},c \mid \mathbf{r} \mid \mathbf{k},v \rangle = \langle \mathbf{k},c \mid [H_{\rm SCF},\mathbf{r}] \mid \mathbf{k},v \rangle / [E_c(\mathbf{k}) - E_v(\mathbf{k})] \ . \quad (14)$$

The local part of the self-consistent potential commutes with $\mathbf{r}$: the commutator is thus the sum of two terms, coming from kinetic energy and nonlocal bare potential $V_{\rm nl}$. Equation (13) finally reads as

$$\langle \mathbf{k}+\mathbf{q},c \mid e^{i\mathbf{q}\cdot\mathbf{r}} \mid \mathbf{k},v \rangle \simeq \mathbf{q}\cdot\langle \mathbf{k},c \mid (\mathbf{p} - i[\mathbf{r},V_{\rm nl}]) \mid \mathbf{k},v \rangle / [E_c(\mathbf{k}) - E_v(\mathbf{k})] \ . \quad (15)$$

The matrix elements of the commutator $[\mathbf{r},V_{\rm nl}]$ have to be explicitly evaluated: we only notice here that they are well defined even within Born—von Kármán boundary conditions.

With the cautions exposed above, the long-wavelength limits needed to study microscopic dielectric properties can be evaluated analytically even in presence of nonlocal ionic potentials. No finite-$\mathbf{q}$ calculation is performed in the present work.

We stress that the dielectric matrix evaluated here is perfectly consistent with the use of nonlocal ionic pseudopotentials, provided the perturbations considered are induced by *local* potentials. This is indeed our case, which concerns macroscopic electrostatics. When the perturbation is described by a nonlocal potential (as it would be the case in lattice dynamics) the standard dielectric matrix does not contain all the necessary information.

III. CALCULATIONS

The electronic ground state of Si is calculated within DFT, making use of the LDA. The electron-gas data used here as input for the LDA are those by Ceperley and Alder[16] as interpolated by Perdew and Zunger.[17] We use *ab initio* norm-conserving pseudopotentials.[18] Recent work[19] has demonstrated the practical equivalence of the results from either *ab initio* pseudopotential calculations or all-electron ones. Therefore the pseudopotential approach is essentially not an approximation, but a convenient mathematical device which allows the use of plane-wave basis sets. The bare ionic pseudopotentials are generated according to the procedure described in Ref. 20. The explicit expression for Si is

$$V_{\rm ion}(\mathbf{r}) = -(Z_v/r)\,{\rm erf}(r/r_{co}) + \sum_l \hat{P}_l (a_l + b_l r^2) e^{-(r/r_l)^2} , \quad (16)$$

where $\hat{P}_l$'s are projectors over the spaces of l angular momentum wave functions, and the numerical values of the parameters are reported in Table I. The kinetic-energy cutoff used to truncate the plane-wave basis set is 14 Ry, which corresponds to about 250 plane waves at a general point of the Brillouin zone. In Table II we compare some calculated ground-state properties with the corresponding observed values. The agreement is excellent and of the same quality as found by different authors.[4,5]

The electronic self-consistent band structure so calculated is used as input for the calculation of the dielectric matrix. The independent-electron polarizability χ_0 has been evaluated from Eq. (1) using the special-point technique for the BZ integration,[21,22] while the $f_{\rm xc}$ operator is straightforwardly obtained from the self-consistent electronic charge density. We find that fully converged results are obtained using χ_0 and $f_{\rm xc}$ matrices of order 181.

The numerical evaluation of the sum over conduction bands and of the BZ integration in Eq. (1) deserves some particular comments. As a general rule, the "body" matrix elements ($\mathbf{G}$ and $\mathbf{G}' \neq 0$) converge fast with the number of special points and slowly with the number of conduction bands, while the opposite is true for the "head" ($\mathbf{G}=\mathbf{G}'=0$); as for the "wing" matrix elements ($\mathbf{G}$ or $\mathbf{G}'=0$), their convergence behavior is intermediate. Such trends have been already stressed by Baldereschi and Tosatti,[23] who used an empirical pseudopotential scheme. The convergence properties of χ_0 can be easily understood in terms of the energy denominators appearing in Eqs. (1) and (15). Let us write, e.g., the explicit expression for the head of χ_0 in the $\mathbf{q}\to 0$ limit as

$$\chi_0(\mathbf{q},\mathbf{q}) \simeq -\frac{4q^2}{(2\pi)^3} \sum_{v_1,c} \int_{\rm BZ} d\mathbf{k} \frac{|\langle \mathbf{k},c \mid (\mathbf{p} - i[\mathbf{r},V_{\rm nl}]) \mid \mathbf{k},v \rangle|^2}{[E_c(\mathbf{k}) - E_v(\mathbf{k})]^3} \ . \quad (17)$$

TABLE I. Pseudopotential parameters (a.u.) entering Eq. (16), obtained from von Barth and Car, Ref. 20.

l	a_l	b_l	r_l
0	10.152 68	−5.239 25	0.81
1	2.817 88	−1.168 49	0.92
≥2	−5.113 54	1.327 20	1.00

$Z_v = 4, \quad r_{co} = 1.09$

TABLE II. Some properties of the electronic ground state of Si as calculated in the present work. Experimental values are shown for comparison.

	This work	Expt.	Units
Lattice constant	10.25	10.26	a.u.
Bulk modulus	0.96	0.99	MBar
LTO(Γ) phonon frequency	15.5	15.7	THz

TABLE III. Convergence of the calculated value of $\epsilon_{RPA}(0,0)$ with respect to both the number of special points used for BZ integration and the cutoff (Ry) used in the summation over conduction states. The value labeled ∞ has been obtained using 210 conduction states. The difference between two given lines is almost constant, thus showing that the contribution of conduction states higher than 2 Ry is well converged already with 10 points.

Cutoff	10 pts.	28 pts.	60 pts.
2	14.2119	13.4849	13.4035
3	14.2957	13.4885	13.4071
4	14.2971	13.4900	13.4086
10	14.298 46		
∞	14.298 51		

It is easily seen that the quantity $1/[E_c(\mathbf{k})-E_v(\mathbf{k})]^3$ goes rapidly to zero as the band index c increases, but when c runs over the lowest conduction bands, small changes in the energy denominator determine large variations in the integrand, thus making the numerical integration rather precarious. As for the wing elements, they have a squared energy denominator, while for the body elements the energy difference comes in only to the first power, thus explaining the different convergence behavior.

In the present work we have obtained fully converged results summing over 210 conduction bands for all the matrix elements of χ_0. The calculated value of ϵ_∞ is dominated by the head of χ_0, Eq. (17), whose contributions from the lowest conduction bands have to be integrated rather accurately over the BZ. We have used 60 Chadi-Cohen special points[21,22] for conduction bands up to 4 Ry, while contributions from conduction bands above this limit have been integrated using 10 such special points. Convergence studies have been performed either by truncating the sum over conduction states or using 28 special points.[22] The relevant figures, which are reported in Tables III and IV, show that the accuracy of our calculated value of ϵ_∞ is better than 1%, while the use of 10 special points throughout yields a value of ϵ_∞ 7% higher than the converged result.

IV. RESULTS AND DISCUSSION

Our results for the (0,0) element of the direct and inverse dielectric matrices are reported in Table V, both in RPA and in LDA. First of all we notice that, according to our previous discussion, local-field effects lower ϵ_∞ by 10—15%. This is about the same as found in previous calculations performed in different pseudopotential schemes.[23,24]

TABLE IV. Convergence of the calculated value of $\epsilon_\infty(\mathrm{RPA})=1/\epsilon^{-1}_{\mathrm{RPA}}(0,0)$ with respect to the size N of the dielectric matrix which is inverted.

N	ϵ_∞ (RPA)	N	ϵ_∞ (RPA)
27	12.3948	89	12.0442
51	12.1650	113	12.0402
65	12.0514	181	12.0395

TABLE V. Calculated values of the static dielectric constant of Si. First line, obtained from Eq. (3); second line obtained from Eq. (4); experimental data obtained from Refs. 25 and 26.

	$\epsilon(0,0)$	$1/\epsilon^{-1}(0,0)$
RPA	13.41	12.04
LDA	15.17	12.72
Expt.		11.4

The effect of xc, on the contrary, is to increase both ϵ_∞ and $\epsilon(0,0)$. We notice that, contrary to our results and our previous discussion, a null or negative shift for $\epsilon(0,0)$ has been recently reported in a different LDA calculation.[10]

The calculated value of the macroscopic dielectric constant is 12.7, compared to an experimental value of 11.4.[25,26] The theoretical value is therefore 12% off the experiment. So far[4,5] a better agreement between theory and experiment (of the order of a few percent only) has been found for most electronic ground-state properties (see, e.g., Table I). The theory predicts a higher dielectric constant than experiment. The expressions used for xc within LDA are electron-gas based: it is not unlikely that the electronic system shows too high a value of ϵ_∞ as a memory of this metallic parentage.

It may appear surprising that several other properties which crucially depend on dielectric screening are predicted by LDA to a better accuracy than the value of ϵ_∞. Let us consider, e.g., the optical phonon at the zone center.[27,28] In a nonpolar material the microscopic expression of the dynamical matrix[29] does not depend upon the head and wings of the IDM. The present results on ϵ_∞, together with the higher accuracy achieved by LDA in lattice dynamics, show that such approximation performs better in dealing with the microscopic response (body of the IDM) than with the macroscopic one (head and wings).

From a technical point of view, another important difference from other LDA calculations[4,5] concerns the BZ integration. It turns out that 10 special points are more than sufficient in most circumstances, while in the present calculation a substantially finer mesh was needed to achieve a comparable accuracy.

In conclusion, we have applied for the first time the tools of modern DFT to the calculation of the macroscopic dielectric constant of a semiconductor. The prediction is in good agreement with experiment, although not as good as obtained in other applications of the LDA to covalent materials. The field of macroscopic dielectric properties of semiconductors proves to be a very stringent benchmark not only for numerical techniques, but also for the predictive power of LDA itself.

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