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Ab initio quasiparticle energies in 2*H*, 4*H*, and 6*H* SiC

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Ab initio quasiparticle energies are calculated for the 2*H*, 4*H*, and 6*H* polytypes of SiC within the *GW* approximation for the self-energy. The starting point is a calculation within the pseudopotential local-density approximation framework. The calculated fundamental gaps of 3.15, 3.35, and 3.24 eV for 2*H*, 4*H*, and 6*H* SiC, respectively, show very good agreement with experimental data. The energy dependence of the screened interaction is modeled by a plasmon pole model from which the plasmon band structures are obtained. [S0163-1829(98)04735-3]

I. INTRODUCTION

SiC polytypes are wide-band-gap indirect semiconductors with a relatively large variation in electronic band-gap magnitude, compared to other wide-band-gap materials such as the II-VI compounds ZnS and CdS. In 1964 Choyke *et al.*[1] found, covering seven polytypes of SiC excluding the 2*H* polytype, that the experimental fundamental band gap varies roughly linearly with the degree of hexagonal nature (*h*) for polytypes up to $h = 50\%$. It was recently shown[2,3] that this variation can be very well reproduced in a model that treats the polytypes as different stackings of mutually twisted cubic SiC layers with appropriate boundary conditions at the layer interfaces. The electronic structure of cubic (3*C*, or *β*) SiC is then taken as the starting point. The essential mechanism of the band-gap formation can be described within an even more simple Kronig-Penney–like model.[3,4]

Of course, a more fundamental treatment of the electronic structure should display the same band-gap variation. Indeed, calculations based on the local-density approximation (LDA) of density-functional theory (DFT) show such a variation; see Ref. 5 and references therein. However, the size of the LDA gaps is much too low due to a nowadays well-known deficiency of DFT.[6] This deficiency can be cured by replacing the local and energy-independent exchange-correlation potential within DFT by a nonlocal energy-dependent self-energy obtained within the *GW* approximation.[6–11] Such an approach was followed for the cubic polytype of SiC leading to excellent agreement with experiment.[12,13] Wenzien, Käckell, Bechstedt, and Cappellini[14] (WKBC) have performed simplified *GW* calculations for 3*C*, 2*H*, 4*H*, and 6*H* SiC. The simplifications involve the use of a model dielectric function and an approximate treatment of the so-called local-field effects. The resulting fundamental gaps, calculated at the theoretical lattice constants, show good agreement with experiment for 3*C* and 6*H* SiC, while the agreement is reasonable for 4*H* and 2*H* SiC: 3.68, 3.56, 3.25, and 2.59 eV for 2*H*, 4*H*, 6*H*, and 3*C* SiC, while experimental values are 3.33, 3.28, 3.10, and 2.42 eV, respectively. The latter values are absorption gaps[1,15] that are, except for 2*H* SiC, corrected for measured exciton binding energies.[16,17]

The aim of the present paper is to perform *GW* calculations for the 2*H*, 4*H*, and 6*H* SiC polytypes without the approximations made in Ref. 14 and to investigate whether

possibly better agreement with experiment can be obtained. Since the fundamental band gaps of the crystals under consideration are accurately known experimentally, such an investigation can shed more light on the reliability of the *GW* method. For the energy dependence of the screened interaction appearing in the *GW* method we utilize a plasmon pole model (PPM), yielding as an interesting by-product the plasmon band structure, which can be subjected to experimental verification.[18] A previous application of this plasmon pole model to 3*C* SiC yielded quasiparticle energies and a lowest plasmon energy in excellent agreement with experiment.[13]

In Sec. II we will give a description of some theoretical and calculational details. In Sec. III we will give the results of the plasmon band structures and *GW* quasiparticle energies. For the latter results we have concentrated on energy levels around the band gap, at specific points in the first Brillouin zone (1BZ) of 2*H*, 4*H*, and 6*H* SiC; see Fig. 1. We conclude briefly in Sec. IV.

II. THEORY

As input to our *GW* calculations we use wave functions and energies $|l,\mathbf{k}\rangle$ and $\varepsilon_l(\mathbf{k})$, respectively, obtained within the framework of the LDA. Here **k** is a wave vector in the 1BZ and *l* is an electron-band index. The closeness of the
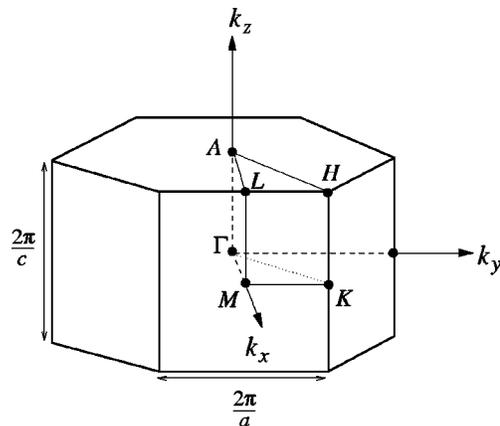

FIG. 1. Hexagonal Brillouin zone, with *a* and *c* the hexagonal lattice constants. Some hexagonal high symmetry points are indicated.

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quasiparticle (QP) wave functions in the GW approximation and the LDA wave functions was demonstrated in various cases[8,9] and we assume that the same is true in the present case, so that we can replace QP by LDA wave functions. Using a first-order expansion of the self-energy operator $\Sigma(\mathbf{k};\varepsilon)$, where ε is the energy, around the LDA energies one finds for the QP energies

$$E_l^{\mathrm{QP}}(\mathbf{k}) = \varepsilon_l(\mathbf{k}) + Z_{l,\mathbf{k}}\langle l,\mathbf{k}| - V^{\mathrm{XC}} + \hbar\Sigma^X(\mathbf{k})$$
$$+ \hbar\Sigma^C(\mathbf{k};\varepsilon_l(\mathbf{k}))|l,\mathbf{k}\rangle, \qquad (1)$$

where $Z_{l,\mathbf{k}}$ is the so-called wave-function renormalization factor, given by

$$Z_{l,\mathbf{k}} = \left(1 - \hbar\langle l,\mathbf{k}|\frac{\partial\Sigma^C(\mathbf{k};\varepsilon)}{\partial\varepsilon}\Big|_{\varepsilon=\varepsilon_l(\mathbf{k})}|l,\mathbf{k}\rangle\right)^{-1}. \qquad (2)$$

In Eq. (1) $\Sigma^X(\mathbf{k})$ is the exchange, or Fock, part of the self-energy operator and $\Sigma^C(\mathbf{k};\varepsilon)$ the energy-dependent correlation part. The exchange-correlation potential V^{XC} can be interpreted as the self-energy in the LDA and hence has to be subtracted in Eq. (1). Within the GW approximation the self-energy is approximated by the product of the electron Green's function G and the screened interaction W (multiplied by i). In line with common practice, we approximate the electron Green's function by the LDA Green's function and evaluate the screened interaction W in the random-phase approximation (RPA). For the energy dependence (ω dependence) of the screened interaction we use the PPM of Engel and Farid.[18] This PPM yields in the limit $\omega \to 0$ the correct static expression for the screened interaction and ensures in the limit $\omega \to \infty$ satisfaction of the Johnson f-sum rule.[19] With these approximations, we find for the correlation part in Eq. (1)

$$\langle l,\mathbf{k}|\hbar\Sigma^C(\mathbf{k};\varepsilon)|l,\mathbf{k}\rangle = \int_{1\mathrm{BZ}}\frac{d^3q}{(2\pi)^3}\sum_{l'\in\mathcal{E}}\sum_{m\in\mathcal{P}}\frac{\left|\sum_{\mathbf{G}}w_{m,\mathbf{q}}^*(\mathbf{G})\sum_{\mathbf{G}'}d_{l',\mathbf{k}-\mathbf{q}}^*(\mathbf{G}'-\mathbf{G})d_{l,\mathbf{k}}(\mathbf{G}')\right|^2}{\varepsilon - \varepsilon_{l'}(\mathbf{k}-\mathbf{q}) + [\omega_m(\mathbf{q})-i\eta]\mathrm{sgn}[\mu-\varepsilon_{l'}(\mathbf{k}-\mathbf{q})]}. \qquad (3)$$

In this expression, $\mathcal{E}$ denotes the electron bands, $\mathcal{P}$ denotes the plasmon bands, η is an infinitesimally small positive energy, and μ is the chemical potential, which in the case of a semiconductor is situated in the energy gap. The $d_{l,\mathbf{k}}(\mathbf{G})$ ($\mathbf{G}$ is a reciprocal lattice vector) denotes a plane-wave coefficient of the LDA wave functions. The plasmon coefficients $w_{m,\mathbf{q}}(\mathbf{G})$ and energies $\omega_m(\mathbf{q})$ follow from a generalized eigenvalue problem.[18] Contrary to other plasmon pole models, which merely serve to give an analytic approximation of the energy dependence of the screened interaction, the plasmon energies of the PPM used can be interpreted physically, at least for the lowest-lying plasmon bands.[18] If nonlocal pseudopotentials are used, as we have done, it can be shown that the f-sum rule is not exactly obeyed.[20] However, in Ref. 21 it has been concluded that this violation has only a minor effect on QP energies.

In the numerical implementation, wave-vector integrations such as in Eq. (3) are replaced by discrete sums. These summations will be performed over the grid

$$\mathbf{q} = (n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3)/2N_{\mathrm{gr}} \quad (n_i = -N_{\mathrm{gr}}+1,\ldots,N_{\mathrm{gr}}), \qquad (4)$$

with $\mathbf{q}$ reduced to the 1BZ if necessary. The $\mathbf{b}_i$ are the primitive vectors of the reciprocal lattice. The integrands of the contributions from Σ^X and Σ^C [see Eq. (3) for the expectation value of the latter] have a singularity if the wave vector in the Brillouin zone integration vanishes ($\mathbf{q} \to \mathbf{0}$). This singularity is integrable and is handled analytically in a way similar to that described in Appendix B of Ref. 22. The only difference is that in the calculation of the contribution of the singular part of the integrand instead of a spherical region an ellipsoidal region is used, which is better adapted to the hexagonal unit cells of the crystals under consideration.

The static dielectric constant ϵ_∞ is defined by $\epsilon_\infty = 1/\lim_{\mathbf{q}\to 0}\{\epsilon^{-1}(\mathbf{q};\omega=0)\}_{\mathbf{G}=0,\mathbf{G}'=0}$, where ϵ is the dielectric matrix and is anisotropic in the case of hexagonal symmetry: The transversal (i.e., perpendicular to the c or k_z axis of the hexagonal Brillouin zone) static dielectric constant $\epsilon_{\perp\infty}$ is generally not equal to the longitudinal (i.e., parallel to the c or k_z axis) static dielectric constant $\epsilon_{\parallel\infty}$. For instance, for $6H$ SiC the experimental values are 6.52 and 6.70, respectively, while for $3C$ SiC the isotropic value of 6.52 applies.[23] In the simplified GW scheme of WKBC some anisotropic effects of the static dielectric constants were incorporated: The available transversal and longitudinal static dielectric constants of $6H$ and $3C$ SiC were used to obtain the ones for $2H$ and $4H$ SiC by extrapolation as a function of h. However, it is not evident that the dielectric constants of hexagonal polytypes should vary linearly with h. We use *ab initio* LDA RPA dielectric matrices as input. In principle, the anisotropy in the limit $\mathbf{q} \to \mathbf{0}$ in the integrand of Eq. (3) could be dealt with. However, because of the fact that the anisotropy is small (for $6H$ SiC, for instance, it is about 3%) we ignore it altogether and calculate the dielectric matrix and the screened interaction for $\mathbf{q} \to \mathbf{0}$ in one particular direction. In order to check the validity of this procedure we have investigated the dependence of the calculated QP energies upon this direction and concluded that it is negligible for the materials under consideration.

III. RESULTS

In our calculations we used energies and wave functions obtained from well-converged pseudopotential LDA calculations carried through in a plane-wave basis set with a cutoff of 50 Ry, corresponding to the number of plane waves N_{PW} of 1689, 3355, and 5057 for $2H$, $4H$, and $6H$ SiC, respec-
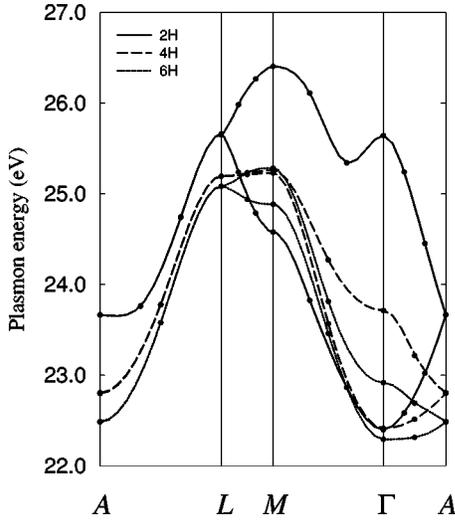
FIG. 2. Calculated dispersion of the two lowest-lying plasmon bands along some symmetry axes of the hexagonal 1BZ (see Fig. 1). The filled circles indicate the actually calculated values. The plotted plasmon energies at Γ were obtained by taking the zero-wave-vector limit along the Γ-A axis.

tively. To calculate the charge density from the wave functions eight special points in the full irreducible wedge of the 1BZ were used, generated according to Pack and Monkhorst.[24] We used the experimental hexagonal lattice constants[23] $a = 3.0763$ Å and $c = 5.0480$ Å for 2*H* SiC, $a = 3.073$ Å and $c = 10.053$ Å for 4*H* SiC, and $a = 3.0806$ Å and $c = 15.1173$ Å for 6*H* SiC. The distance between the Si and C atom in each Si-C pair was taken equal to the ideal value $3c/4p$ for the polytype pH. The deviations from this ideal value are less than 0.3%.[5,25] The implemented parametrization of the *ab initio* nonlocal ionic norm-conserving pseudopotentials was that of Bachelet, Greenside, Baraff, and Schlüter.[26] The exchange-correlation potential V^{XC} was represented with the Wigner interpolation formula.[27]

In the calculation of the expectation values and their energy derivatives of the correlation part and the expectation values of the exchange part of the GW self-energy [see Eqs. (1)–(3)] the number of **q** points in the wave-vector summations [see Eq. (4)] was taken to be 216 ($N_{gr} = 3$) for 2*H* and 64 ($N_{gr} = 2$) for 4*H* and 6*H* SiC. In the calculation of the RPA dielectric matrices the same numbers were used, except for the zero-wave-vector limit in the case of 2*H* SiC for which the number of **q** points was taken to be 512 ($N_{gr} = 4$). In the calculation of the RPA dielectric matrices and the expectation values and their energy derivatives of the correlation part of the self-energy, both N_{PW} and the numbers of electron bands (and plasmon bands in the latter case) taken into account were 287, 563, and 851 for 2*H*, 4*H*, and 6*H* SiC, respectively. In the calculation of the expectation values of the exchange part of the self-energy and the exchange-correlation potential in Eq. (1) we took $N_{PW} = 391$, 813, and 1211 for 2*H*, 4*H*, and 6*H* SiC, respectively. With these cutoffs our calculated QP and plasmon energies are converged to within 0.05 eV for 2*H* SiC and 0.1 eV for 4*H* and 6*H* SiC. The **q**$\rightarrow$**0** limit of the dielectric matrix and screened interaction was taken along the Γ-A axis (see Fig.
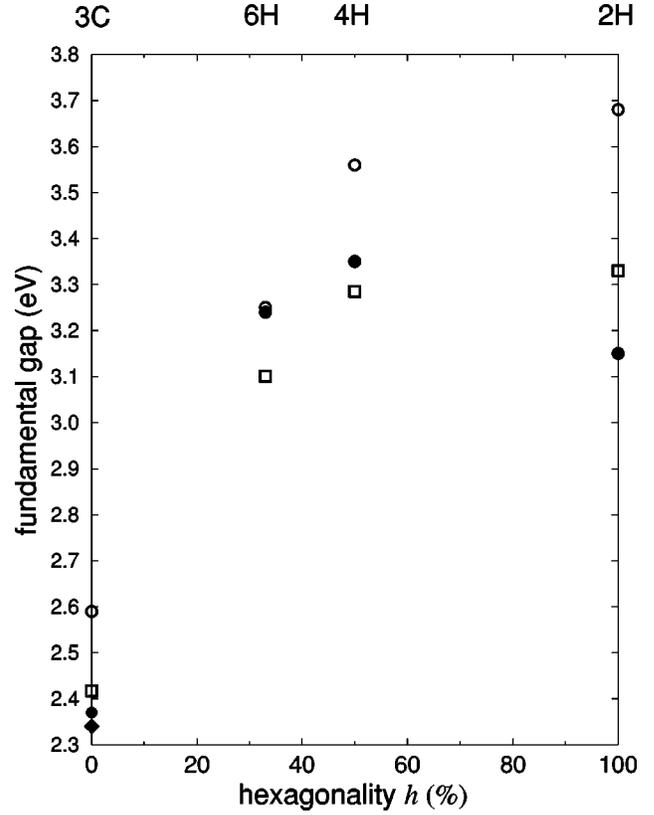
FIG. 3. Fundamental gap versus percentage hexagonality (h). The results of the present study and the result of Ref. 13 for 3*C* SiC are indicated by filled circles. The result of Ref. 12 for 3*C* SiC is indicated by a diamond. Results reported by WKBC are indicated by open circles. The experimental values, corrected for the exciton binding energies (except for 2*H* SiC; see the main text), are plotted as squares.

1). For 2*H* SiC we have investigated the influence of the anisotropy of the dielectric function on our calculated GW quasiparticle energies by taking **q**$\rightarrow$**0** along other directions than Γ-A. The resulting deviations in the GW quasiparticle energies were only about 0.02 eV. The effects of anisotropy in 4*H* and 6*H* SiC are expected to be even smaller. As a test of our computer code we recalculated the QP and plasmon energies of 3*C* (cubic) SiC in the hexagonal 6*H* unit cell and checked our results against those of Ref. 13.

In Fig. 2 we have plotted for 2*H*, 4*H*, and 6*H* SiC the two lowest-lying plasmon bands (obtained from the generalized eigenvalue problem of Ref. 18) as a function of the wave vector at the high symmetry axes A-L-M-Γ-A in the 2*H*, 4*H*, and 6*H* 1BZ, respectively. The lowest plasmon energy, which occurs at Γ, is shown to vary barely with the polytype: 22.40, 22.42, and 22.30 eV for 2*H*, 4*H*, and 6*H* SiC, respectively. Only one experimental value of the lowest plasmon energy for both 3*C* SiC and noncubic polytypes of SiC is known to us, namely, 22.1 eV.[28] The calculated values agree well with this experimental value. It would be interesting to compare our plasmon dispersions with experimental data. However, as far as we know, measurements of plasmon dispersions for the SiC polytypes have not yet been reported on in the literature.

Our LDA and QP energies for 2*H*, 4*H*, and 6*H* SiC for the highest valence band and the lowest conduction band at

TABLE I. Quasiparticle energies (in eV) at some high symmetry points of the hexagonal Brillouin zone for $2H$, $4H$, and $6H$ SiC. Results of the present study (also the LDA results are given) as well as those of WKBC are included. The included experimental energies are corrected for exciton binding energies (except for $2H$ SiC; see the main text). All energies refer to the valence-band top (Γ_{6v}), which is set at 0 eV.

$l,\mathbf{k}$	6H				4H				2H			
	LDA	Present	WKBC	Expt.	LDA	Present	WKBC	Expt.	LDA	Present	WKBC	Expt.
Γ_{6v}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Γ_{1c}	5.10	6.57	6.95		5.15	6.44	6.92		4.81	5.83	6.66	
K_{2v}									-3.84	-4.07	-4.12	
K_{2c}									2.01	3.15	3.68	3.33
H_{3v}									-1.67	-1.83	-1.83	
H_{3c}									4.99	6.13	6.86	
$A_{5,6v}$	-0.08	-0.09	-0.09		-0.20	-0.22	-0.20		-0.70	-0.78	-0.75	
$A_{1,3c}$	5.17	6.64	7.02		5.36	6.65	7.14		5.90	6.96	7.81	
M_{4v}	-1.04	-1.11	-1.40		-1.06	-1.15	-1.23		-1.14	-1.25	-1.13	
M_{1c}	1.82	3.24	3.25	3.10	2.08	3.35	3.56	3.28	2.57	3.67	4.28	
$L_{1,2,3,4v}$	-1.23	-1.33	-1.63		-1.50	-1.61	-1.68		-2.29	-2.48	-2.30	
$L_{1,3c}$	1.85	3.29	3.36		2.49	3.80	4.06		3.16	4.23	4.85	

some high symmetry points in the 1BZ are listed in Table I, together with the corresponding results of WKBC and the experimental data. It is known that in $6H$ SiC a camel's back structure for the lowest conduction band along the L-M axis exists, but, based on the results of Ref. 29, we assume that taking the lowest conduction band at the M point leads only to a minor error in the calculated GW fundamental gap for $6H$ SiC. Our calculated GW fundamental band gaps are 3.15, 3.35, and 3.24 eV for $2H$, $4H$, and $6H$ SiC, respectively. In comparing these gaps with the absorption gaps of 3.330 eV for $2H$ SiC (Ref. 15) and 3.263 and 3.023 eV for $4H$ and $6H$ SiC, respectively,[1] we have to account for the exciton binding energies. For $4H$ and $6H$ SiC these binding energies are experimentally found to be 0.020 and 0.078 eV, respectively,[16,17] i.e., smaller than the accuracy of our GW calculations. For $2H$ SiC no value for the exciton binding energy is known to us, but it is hard to believe that the value for this binding energy would be larger than the above-mentioned values. The agreement between our results and the experimental results is very good. The largest difference is found for $2H$ SiC: 0.18 eV. In Fig. 3 we have collected fundamental gap values of the present work, of WKBC, of Rohlfing et al.[12] and of Backes et al.[13] and the experimental fundamental gaps in a plot of gap versus h. It is clearly seen that the results of the simplified GW calculations of WKBC are in general not as good as those of the more rigorous calculations of the present work and Refs. 12 and 13. For $6H$ SiC (one of the polytypes for which WKBC applied the model dielectric function using the available experimental dielectric constants) the result with regard to the fundamental gap is of comparable quality. Concerning the GW values of indirect gaps other than the fundamental gaps, the differences between the results of WKBC and the present work are

larger than for the fundamental gaps. It would be interesting to compare the calculated values with experimental values for these other indirect gaps, but we are not aware of such measurements.

As far as dielectric constants are concerned, we can only report a reliable value for the longitudinal dielectric constant $\epsilon_{\parallel\infty}$ of $2H$ SiC: 7.23. This value agrees very well with the theoretical value 7.32 reported in Ref. 30, in which a more systematic study of the dielectric properties of SiC polytypes was performed, and the theoretical value 7.28 reported in Ref. 31.

IV. CONCLUSION

Summarizing, ab initio plasmon band structures and GW quasiparticle energies have been presented for the $2H$, $4H$, and $6H$ polytypes of SiC. Our GW quasiparticle energies improve those of previous simplified GW calculations and are in very good agreement with experimental values. It has been demonstrated that the GW approximation yields reliable predictions of quasiparticle energies also for this class of materials.

ACKNOWLEDGMENTS

[1] W. J. Choyke, D. R. Hamilton, and L. Patrick, Phys. Rev. **133**, A1163 (1964).

[2] W. H. Backes, P. A. Bobbert, and W. van Haeringen, Phys. Rev. B **49**, 7564 (1994).

[3] W. van Haeringen, P. A. Bobbert, and W. H. Backes, Phys. Status Solidi B **202**, 63 (1997).

[4] W. H. Backes, F. C. de Nooij, P. A. Bobbert, and W. van Haeringen, Physica B **217**, 207 (1996).

[5] P. Käckell, B. Wenzien, and F. Bechstedt, Phys. Rev. B **50**, 10 761 (1994).

[6] R. W. Godby, M. Schlüter, and L. J. Sham, Phys. Rev. Lett. **56**, 2415 (1986); Phys. Rev. B **35**, 4170 (1987).

[7] L. Hedin, Phys. Rev. **139**, A796 (1965).

[8] M. S. Hybertsen and S. G. Louie, Phys. Rev. Lett. **55**, 1418 (1985); Phys. Rev. B **34**, 5390 (1986).

[9] R. W. Godby, M. Schlüter, and L. J. Sham, Phys. Rev. B **37**, 10 159 (1988).

[10] W. von der Linden and P. Horsch, Phys. Rev. B **37**, 8351 (1988).

[11] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998).

[12] M. Rohlfing, P. Krüger, and J. Pollmann, Phys. Rev. B **48**, 17 791 (1993).

[13] W. H. Backes, P. A. Bobbert, and W. van Haeringen, Phys. Rev. B **51**, 4950 (1995).

[14] B. Wenzien, P. Käckell, F. Bechstedt, and G. Cappellini, Phys. Rev. B **52**, 10 897 (1995); B. Wenzien, G. Cappellini, and F. Bechstedt, *ibid.* **51**, 14 701 (1995).

[15] L. Patrick, D. R. Hamilton, and W. J. Choyke, Phys. Rev. **143**, 526 (1966).

[16] V. I. Sankin, Sov. Phys. Solid State **17**, 1191 (1975).

[17] G. B. Dubrovskii and V. I. Sankin, Sov. Phys. Solid State **17**, 1847 (1975).

[18] G. E. Engel and B. Farid, Phys. Rev. B **47**, 15 931 (1993).

[19] D. L. Johnson, Phys. Rev. B **9**, 4475 (1974).

[20] G. E. Engel and B. Farid, Phys. Rev. B **46**, 15 812 (1992).

[21] R. T. M. Ummels, P. A. Bobbert, and W. van Haeringen, Phys. Rev. B **57**, 11 962 (1998).

[22] R. Daling and W. van Haeringen, Phys. Rev. B **40**, 11 659 (1989).

[23] *Semiconductors: Physics of Group IV Elements and III-V Compounds*, edited by K.-H. Hellwege and O. Madelung, Landolt-Börnstein, New Series, Group III, Vol. 17, Pt. a (Springer-Verlag, Berlin, 1982).

[24] J. D. Pack and H. J. Monkhorst, Phys. Rev. B **16**, 1748 (1977).

[25] F. Bechstedt, P. Käckell, A. Zywietz, K. Karch, B. Adolph, K. Tenelsen, and J. Furthmüller, Phys. Status Solidi B **202**, 35 (1997).

[26] G. B. Bachelet, H. S. Greenside, G. A. Baraff, and M. Schlüter, Phys. Rev. B **24**, 4745 (1981).

[27] E. P. Wigner, Phys. Rev. **46**, 1002 (1934).

[28] H. Raether, *Excitation of Plasmons and Interband Transitions by Electrons*, edited by G. Höhler, Springer Tracts in Modern Physics Vol. 88 (Springer, Berlin, 1980).

[29] W. R. L. Lambrecht, S. Limpijumnong, S. N. Rashkeev, and B. Segall, Phys. Status Solidi B **202**, 5 (1997).

[30] J. Chen, Z. H. Levine, and J. W. Wilkins, Phys. Rev. B **50**, 11 514 (1994).

[31] K. Karch, F. Bechstedt, P. Pavone, and D. Strauch, Phys. Rev. B **53**, 13 400 (1996).