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Semiempirical self-energy corrections to LDA bands of semiconductors, and a scaling law for the scissor operator

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Abstract. A semiempirical approach to the evaluation of corrections to LDA electronic states and effective masses in semiconductors is described. Applications to GaAs, AlAs, Ge, $Ga_{1-x}Al_xAs$ VCA alloys are presented, and a scaling law for the scissor operator is discussed.

1. Introduction

The local density approximation (LDA) to density functional theory (DFT) [1] is a very successful method for calculating electronic and structural properties of solids. Computational procedures based on the LDA, though, are known to underestimate the band gaps of semiconductors systematically [2, 3]; this problem has been shown to be intrinsic to DFT itself [1, 4, 5]. The description of the excited states in a crystal requires the computation of the quasiparticle (QP) spectrum of the system, i.e. the solution of a self-consistent one-body equation involving the energy-dependent, non-local electron self-energy, an operator that is generally constructed to lowest order in many-body perturbation theory in the GW approximation of Hedin [6, 7].

GW calculations have provided impressive progress [5, 8], but they are very elaborate and time-consuming as compared to the LDA; such are also, although to a lesser degree, the approximate approaches of [9, 10] to computing self-energy corrections to LDA electronic states. Furthermore, once applied to the bulk materials, none of these techniques are easily 'exportable' to more complex related systems, either because of the specific approximations involved (in the case of models), or the sheer computational load (as for full calculations). It is thus desirable to devise some simpler technique to estimate self-energy corrections to LDA eigenvalues in bulk solids and related systems.

In the present work we discuss a semiempirical approach to the problem. The focus is on correcting the LDA bands in a class of materials by a procedure that incorporates as much as possible of the relevant physics (long-range, dielectric screening, energy dependence), with the goal of precise ($\delta \simeq 0.01$–0.05 eV) eigenvalues and related properties (say masses), simplicity, rapidity, and transferability to more complex systems (alloys, superlattices).

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2. Method

The leading term in the many-body expansion of the self-energy in powers of the screened interaction—that is, the GW form of the self-energy—is [6, 5]

$$\Sigma^{\mathrm{GW}}(r, r', E) = \frac{\mathrm{i}}{4\,\pi} \int \mathrm{e}^{\mathrm{i}\omega\delta} G(r, r'; E + E') W(r, r'; E') \, \mathrm{d}E' \tag{1}$$

with δ an infinitesimal number, G the one-electron Green's function and W the effective screened interaction. The spatial range of this quantity is determined by the potential W; while in metals the Coulomb interaction is well screened and the potential decays rapidly as $|r - r'| \to \infty$ (in the RPA, $W \simeq r^{-3}$ times Friedel oscillations) and the self-energy is short-ranged [1, 7], in semiconductors $W \to 1/(\varepsilon_\infty |r - r'|)$ in the same limit, due to the incomplete screening of the Coulomb interaction [10]. In the case of insulators we may then decompose W into a short-ranged metal-like part (whence one recovers the local exchange-correlation potential of the inhomogeneous electron gas $V_{\mathrm{xc}}^{\mathrm{LDA}}$, if its weak energy dependence is neglected), and a long-ranged part, small as $|r - r'| \to 0$ and with the above long-range behaviour. The expectation value of the self-energy part related to this term, $\delta\Sigma$, is known to be discontinuous across the energy gap [5, 8, 10, 11]. The goal of the present work is then to reproduce $\delta\Sigma$, the slowly varying long-ranged correction to $V_{\mathrm{xc}}^{\mathrm{LDA}}$, by means of a smooth non-local potential.

The technique is as follows. The equilibrium structure and volume of the bulk crystal are determined *ab initio* by a converged LDA [12] pseudopotential [13] plane-wave calculation (using 10 special k-points [14] and a cut-off of 20 Ryd) and the electronic eigensystem is computed at a set M of additional selected k-points (Γ, X, L in the present case). We then solve the eigenvalue problem for the 'empirical quasi-particle' (EQP) Hamiltonian $H = H_{\mathrm{LDA}} + V_{\mathrm{E}}$, expanding the EQP eigenstates on the basis of LDA eigenstates. H_{LDA} is the self-consistent LDA Hamiltonian, and the non-local potential V_{E} is a sum of local potentials projected onto occupied (valence) and virtual (conduction) states:

$$V_{\mathrm{E}} = V_{\mathrm{E}}^v P_v + V_{\mathrm{E}}^c (1 - P_v) \tag{2}$$

with $P_v = \sum_v |vk\rangle\langle vk|$ the projector on the LDA valence manifold. V_{E}^c is expanded in Fourier space as

$$V_{\mathrm{E}}^c(r) = \sum_G V_{\mathrm{E}}^c(G) S(G) \mathrm{e}^{\mathrm{i}G \cdot r} = \sum_G V_{\mathrm{E}}^{Sc}(G) \mathrm{e}^{\mathrm{i}G \cdot r} \tag{3}$$

($S = \sum_s \mathrm{e}^{\mathrm{i}G \cdot \tau_s}$ is the crystal basis structure factor, the G are reciprocal-lattice vectors, and V_{E}^{Sc} is defined by the second equality), and analogously for V_{E}^v.

The matrix elements of H between LDA eigenstates (mk) and (nk) are

$$A_{m,n} = \sum_{G,G'} C_{m,k}^*(G) C_{n,k}(G') V_{\mathrm{E}}^{Si}(G - G') + E_{n,k}^{\mathrm{LDA}} \delta_{m,n} \tag{4}$$

where $m, n = 1, \ldots, N$ are band indices, C the coefficients of the plane-wave expansion of the LDA wavefunction at a specific k-point, and G, G' are reciprocal-lattice vectors. Matrix elements between conduction and valence states are zero by construction, so in (4) the label i stands for either c or v.

While N is fixed for valence, when dealing with conduction states an appropriate truncation $N = N_c$ of the expansion of EQP functions on LDA states must be chosen; since the potential turns out to be quite weak, couplings of the states of interest with bands much higher in energy become rapidly negligible, and $N = N_c \simeq 10$ is found to be sufficient. The value of N_c should be chosen carefully to avoid artificial splittings of degenerate multiplets. In the present work we typically use $N_c \simeq 25$–30 depending on k and degeneracies.

The Fourier components $V_E(G)$ are determined by the requirement that the computed eigenvalues be equal to the corresponding experimental values within experimental error (see below); this amounts to a multidimensional non-linear optimization process, which can be translated into a minimization problem for an appropriate cost function, as shown below. The latter problem is solved by the robust simplex method of Nelder and Mead [15]. In order to estimate the distance of the experimental band structure from the calculated one (which is a functional of V_E) and to produce the potential V_E minimizing this distance, we use a cost function given by the infinity norm of the calculation-to-experiment error, that is, the maximum weighted deviation of the calculated eigenvalues from the pertaining experimental values,

$$F_c = |e|_\infty = \max_{i \in M} \; w_i \, (E_i^{\text{th}} - E_i^{\text{ex}}). \tag{5}$$

The weight for the ith state is the ratio of a reference experimental error $e_r = \min_{\{i \in M\}} e_i$ to the ith experimental error

$$w_i = (e_r/e_i)^{p_i} \tag{6}$$

with i running over the set M of the relevant states considered in the minimization process (the size of this set is usually restricted by the small number of available experimental data [16]). Very accurate experimental values ($w \simeq 1$) can be overweighted by choosing $p > 1$, our value of p ranging from 1 to 1.1. The computation of the cost function amounts to calculating the eigensystem of the Hamiltonian H on the basis of LDA eigenfunctions, at each of the points of the set M. The eigenenergies are

$$E_i^{\text{th}} \equiv E_{i,\text{EQP}} = E_{i,\text{LDA}} + \langle i_{\text{EQP}} k | V_E | i_{\text{EQP}} k \rangle \simeq E_{i,\text{LDA}} + \langle i_{\text{QP}} k | \delta \Sigma | i_{\text{QP}} k \rangle. \tag{7}$$

Of course, these energies will depend critically on the LDA eigenvalues [3]. The eigenfunctions of $H + V_E$ are the EQP wavefunctions $|i_{\text{EQP}} k \rangle = \sum_j q_j |j_{\text{LDA}} k \rangle$, which we find to closely resemble LDA states, that is

$$|i_{\text{EQP}} k \rangle \simeq |i_{\text{LDA}} k \rangle \simeq |i_{\text{QP}} k \rangle \tag{8}$$

where the second equality between GW QP and LDA states is by now well established [5, 8].

For the cases examined here, the minimization converges to a single point in the parameter space of Fourier coefficients of V_E in a limited number of simplex iterations quite independently of the starting point. Occasional minimization restarts are performed as a check. The computational cost of the whole optimization procedure for a specific bulk material is modest, 500 to 800 CPU seconds on a Cray X/MP for conduction states with the present plane-wave basis size of about 450 in the zincblende

structure and depending on the initial conditions (use of softer pseudopotentials [17] may allow a further reduction of the computational effort).

However, the evaluation of the corrections for a potential determined previously for a specific material is equivalent to a single evaluation of the cost function (that is, of the corrected eigenvalues) which is a matter of less than 1 CPU second per k-point for the present basis. This allows us to compute a good approximation to quasiparticle energies and wavefunctions, and related quantities, at basically no expense with respect to the mother LDA calculation; in fact, while the procedure is only carried out at some selected points in the Brillouin zone, the potential accordingly modifies the band structure everywhere else in the zone.

3. Calculations and results

The materials we focus upon here are GaAs, AlAs and Ge. In view of the reasonable agreement of LDA calculations [2, 3, 5, 8] with GW calculations and experiment for valence states, we set the valence self-energy correction to zero, and concentrate on that pertaining to conduction states. Clearly the procedure is the same for valence states, apart from a readjustment of the global energy zero; owing to the need for a fixed reference zero in the calculation, one cannot estimate constant shifts of the quasiparticle band structure relative to the LDA one, so many-body corrections to LDA valence band tops, relevant to the band offset interface problem, are outside the scope of the present approach.

As anticipated above, the dependence on the LDA energies is crucial, so we take care in fully converging the eigenvalues (the maximum deviation is less than 10 meV for the conduction minimum in GaAs), and choose to work with the crystal at zero pressure, i.e. at the theoretical equilibrium volume $\Omega = \Omega_{th}$. As discussed in [3], this avoids dependence of the eigenvalues on the choice of pseudopotentials and most other details of the LDA calculation.

As a general strategy, given the limited number of experimental data, and the expected long-ranged nature of the potential, we only consider Fourier components of V_E up to the $\langle 200 \rangle$ FCC reciprocal-lattice shell. This is a sound choice dictated by the physical considerations on $\delta\Sigma$ outlined in the previous section, but it is also convenient on the computational side, since it cuts down on parameter space dimensionality and matrix element computation, and it keeps the optimization problem under-determined (fewer data than fitting parameters).

For zincblende and diamond structures, we have then four and two free parameters per material, respectively. The total of ten free parameters for the three materials is well below the number of experimental data: it is nevertheless important to look for possible transferability rules of the potential (or parts thereof) among different materials, which will allow a reduction of the number of free parameters.

Non-trivially, the independent minimizations for each material do nicely reproduce the experimental data (within the respective errors), and show that

(i) the Fourier spectrum of V_E is dominated by the $G = \langle 000 \rangle$ component, the scissor operator Δ, which is of order 0.5–1 eV;

(ii) in Ge the $G \neq 0$ component vanishes (this is a computational finding, and not a symmetry restriction);

(iii) the scissor operator Δ scales as the ratio of the high-frequency dielectric constants; that is, $\varepsilon \times \Delta$ is a constant:

$$\Delta = \alpha/\varepsilon \tag{9}$$

with $\alpha \simeq 9$ eV.

Thus the scissor operators of the different materials are not independent parameters; this reduces the number of free parameters for the three materials to seven (neglecting the vanishing $G = (111)$ component in Ge; the available experimental data number 13).

The scaling law of the scissor operator, equation (9), is a useful rule of thumb which can be applied to obtain reasonably accurate estimates of gaps. In many cases (e.g. for wide gaps), the LDA estimate alone is useless, and this rule provides a correction restoring at least an order-of-magnitude agreement. It turns out in fact that the validity of this rule extends well beyond semiconductors. In figure 1 we show the difference Δ between LDA-calculated and experimental gaps for a number of materials, which shows the rule (9) to hold nicely up to very large gaps. In panel (a) the linear fit of the data versus $1/\varepsilon$ gives $\alpha \simeq 9.3$; in panel (b), which is a blow-up of the semiconductor region, the fit gives $\alpha \simeq 9.1$. The rule is seen to give correct predictions within 10% or less. The LDA calculations are our pseudopotential ones for most semiconductors, whereas all-electron calculations are considered for most wide-gap materials [18]. It should be noted that this finding is most useful in wide-gap materials, and in general in all cases in which the LDA gap error is unambiguously prevailing over other sources of computational inaccuracy; in such cases, a precision of 10% is largely sufficient to give a sensible estimate of the gap. Also, the scissor may be in many instances a reasonable correction to the band structure as a whole, as we found here to be the case for Ge at zero pressure (see [3, 19] for more thorough discussions).

We found out that a result similar to ours (equation (9)) has been independently obtained in a different context by von der Linden *et al* [11], who find that their NFE GW self-energy correction to the fundamental gap of diamond as a function of ε is indeed proportional to $1/\varepsilon$, the value of the proportionality coefficient being $a \simeq 9.0$ eV (extracted from figure 1 of [11] at $\varepsilon = 1$). At the actual physical value of ε, a gap in good agreement with experiment is obtained. QP calculations by Hanke and Sham [20] also show a similar linear behaviour of the gap correction (although the constant is about 20% smaller due to the gap of LiCl, which is still underestimated in [20]). We have also reached a similar conclusion computing the scissor operator in the $q \to 0$ limit of the GW COHSEX approximation. In that limit, the correction to the gap is (equation (8) of [10])

$$\Delta \simeq V_{\mathrm{BZ}}^{-1} \int_0^{k_{\mathrm{BZ}}} 4\pi q^2 W(q)\, \mathrm{d}q = \frac{2}{\pi} \int_0^{k_{\mathrm{BZ}}} \mathrm{d}q(\varepsilon_{\mathrm{S}}^{-1} - \varepsilon_{\mathrm{M}}^{-1}) \tag{10}$$

where V_{BZ} is the Brillouin zone volume, the sum over special points is replaced by an integration over a sphere of volume $V_{\mathrm{BZ}} = 4\pi k_{\mathrm{BZ}}^3/3$, and $\varepsilon_{\mathrm{S}}, \varepsilon_{\mathrm{M}}$ are a model semiconductor dielectric function and the Lindhard dielectric function, respectively. The dependence of the scissor operator on density and dielectric constant is pictured in figures 2(a) and (b), using respectively the dielectric functions of Bechstedt and Del Sole [21], and of Resta [22]. In the latter case, the Thomas–Fermi function is

used instead of the Lindhard one for the electron gas. As expected [23], it turns out that the diagonal dielectric screening is not accurate in highly insulating materials, local fields being neglected altogether; in the low-density regime (typically semiconductors), however, the simplified GW COHSEX scissor agrees with the empirical linear law discussed above, which describes the actual correction quite well. It should be noted that the error bar due to different model dielectric functions is at least of order 10% (the Bechstedt–Del Sole function, however, has been recently shown [24] to give results of quality comparable to the calculation of [10], which used the diagonal of the inverse dielectric matrix).
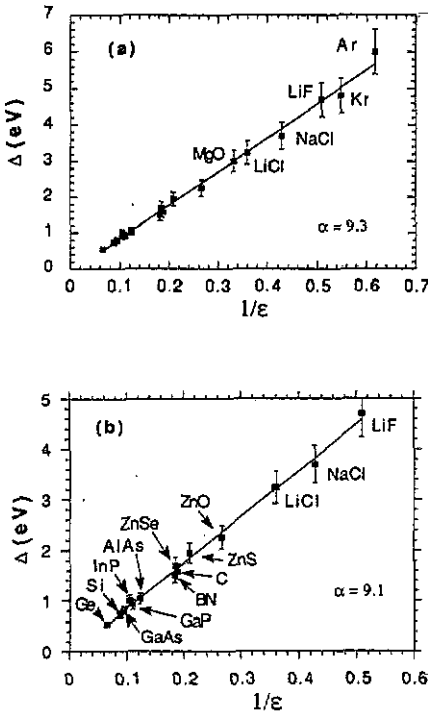

Figure 1. The scaling rule for the scissor operator (panel (a)), and a blow-up of the high-ε region (panel (b)). The data points indicate the scissor operator as determined in the present work; for C, InP, ZnSe, ZnS, ZnO, MgO, LiCl, NaCl, LiF, Kr, Ar the difference between the experimental and computed gaps is plotted instead [18]. Error bars are 10% of the data.
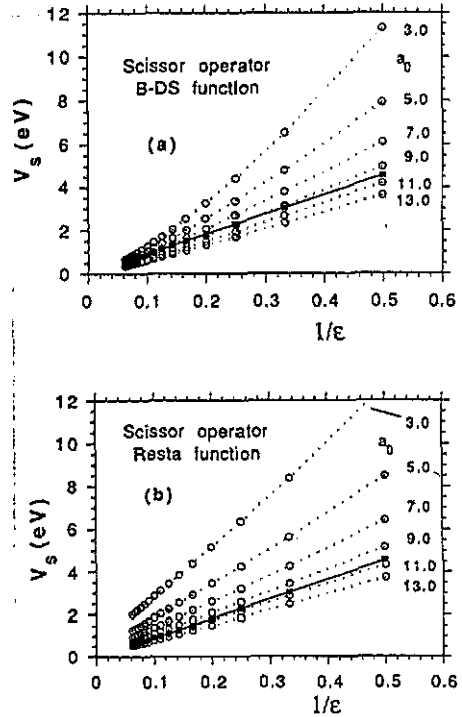
Figure 2. The GW $q \to 0$ scissor operator as a function of $1/\varepsilon$, parametrized by the lattice constant a_0 of the FCC lattice cell for eight electrons, density $= 8/(a_0^3/4)$. In panel (a) the (Lindhard-like) Bechstedt–Del Sole [21] model is used; in panel (b) the (Thomas-Fermi-like) Resta [22] model is used. The empirical rule obtained in the present work is shown as black dots and a continuous line.

The weighted experimental band energies at Γ, X, L determine the potential V_E, which modifies accordingly the bands over the whole Brillouin zone: the LDA and corrected bands along high-symmetry lines are shown in figure 3. The correction to band dispersion also affects other properties: an interesting test is the effective masses (it should be noted that *no information* on effective masses is embedded in the minimization procedure). The computed LDA values of the conduction electron mass [3] in AlAs, GaAs, and Ge at Γ are 0.122, 0.064, and 0.029 at zero pressure.

The correction potential modifies the masses only very slightly: the corrected values are 0.065 (experimental value: 0.0665), 0.125 (experimental value: 0.124) and 0.029 (experimental value: 0.037) for GaAs, AlAs and Ge respectively, in good agreement with experiment [25]. These small corrections, however, result from cancellation of large contributions; this can be seen in figure 4, where the dependence on the different components of the correction potential V_E is shown for the electron effective mass at Γ in GaAs (at Ω_{ex}).
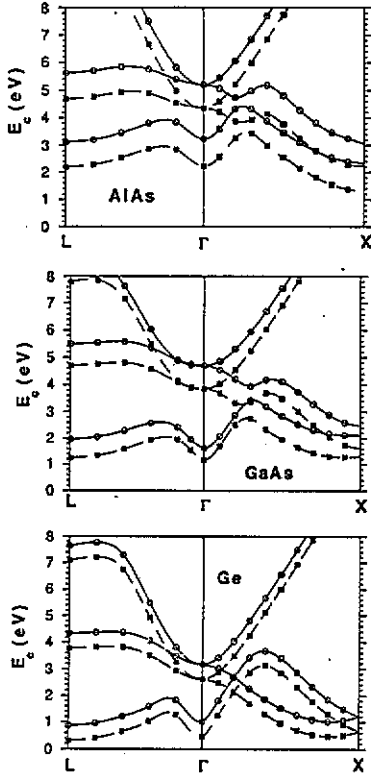

Figure 3. AlAs, Ge and GaAs conduction bands referred to the valence band top. LDA bands are shown by black squares and dashed lines; corrected bands are shown by open circles and solid lines.
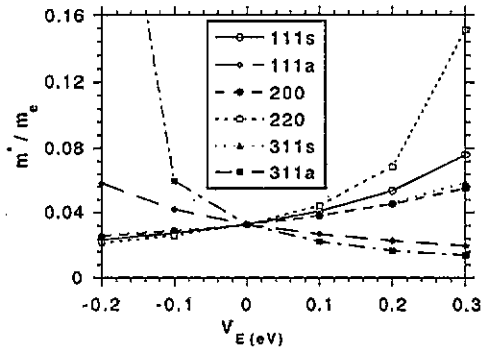
Figure 4. The conduction effective mass at Γ in GaAs as modified by the various symmetric and antisymmetric components of V_E (the basis vectors of the lattice are $\tau_1 = 0$ and $\tau_2 = a_0(1,1,1)/4$).

Finally, the correction potentials obtained for bulk GaAs and AlAs have been applied to the ternary alloy $Al_x Ga_{1-x} As$. A linear interpolation $V_E^{alloy} = x\, V_E^{GaAs} + (1-x)\, V_E^{AlAs}$ is used for V_E. The LDA eigensystem is calculated self-consistently as a function of x in the virtual-crystal approximation; the technicalities are the same as for the bulk. The virtual-crystal lattice constant is interpolated linearly between those of GaAs and AlAs according to Vegard's law, a behaviour confirmed by linear-response-theory supercell calculations [26]. The LDA bands are shown in figure 5(*a*), and the corrected bands in figure 5(*b*). The crossover mole fractions are given in table 1: although the situation is not very satisfactory, it is a vast improvement on the bare LDA case. The $E_c(x)$ relations are found to be essentially linear, the bowing parameters (given in table 2) being an order of magnitude smaller than the

experimental values: this is not unexpected, since the bowings (as well as higher-order effects) are in fact a manifestation of microscopic alloy disorder [26], which is absent in the virtual crystal. The effective mass of electrons at Γ is estimated to change with composition as $m^*(x) = 0.065 + 0.06\,x$.

Table 1. Alloy crossover mole fractions.

Crossing	LDA	Present	Experiment
Γ–X	0.105	0.345	0.405
Γ–L	0.385	0.720	0.432
L–X	0.040	0.155	0.350

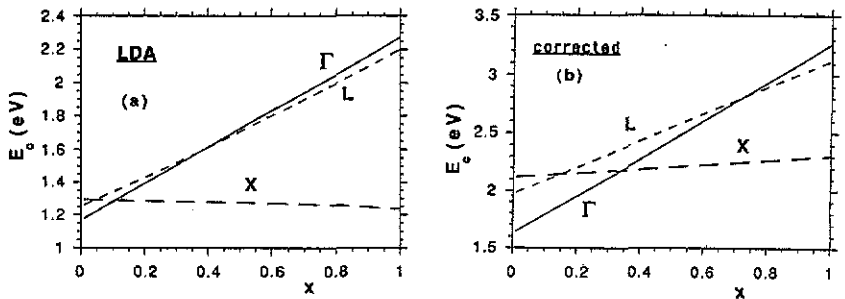**Figure 5.** LDA (panel (a)) and corrected (panel (b)) electronic states at L, Γ, X for a Vegard VCA $Al_x Ga_{1-x} As$ alloy as a function of x.

Table 2. Alloy bowing parameters $C(E(x) = A + Bx + Cx(1 - x))$.

Transition	Present	Experiment
$\Gamma \to L$	−0.001	0.055
$\Gamma \to X$	0.021	0.245
$\Gamma \to \Gamma$	0.025	0.370

4. Conclusions

We have described a simple method for approaching the LDA gap problem in bulk semiconductors and related systems; it amounts to an optimization procedure producing a smooth semiempirical non-local potential, which reproduces the effect of the long-range part of the self-energy associated with incomplete screening in insulators. The technique has been applied to GaAs, Ge, AlAs, and the AlGaAs alloy. An interesting linear scaling rule for the scissor operator versus the dielectric constant has been obtained, which is valid also for wide-gap materials.

Acknowledgment

References

[1] Dreizler R M and Gross E K U 1990 *Density Functional Theory* (Berlin: Springer) and references therein
[2] Hamann D R 1979 *Phys. Rev. Lett.* 42 662
  Bachelet G B and Christensen N E 1985 *Phys. Rev.* B 31 879
[3] Fiorentini V 1992 *Phys. Rev.* B at press; 1992 *Solid State Commun.* submitted
[4] Perdew J P and Levy M 1983 *Phys. Rev. Lett.* 51 1884
  Sham L J and Schlüter M 1983 *Phys. Rev. Lett.* 51 1888; *Phys. Rev.* B 32 3883
[5] Godby R W, Schlüter M and Sham L J 1988 *Phys. Rev.* B 37 10159
[6] Hedin L 1969 *Phys. Rev.* B 139 A796
  Hedin L and Lundqvist S 1969 *Solid State Physics* vol 23 (New York: Academic) p 1
[7] Gunnarsson O and Jones R O 1989 *Rev. Mod. Phys.* 61 689 and references therein
[8] Hybertsen M S and Louie S G 1985 *Phys. Rev.* B 32 7005; 1986 *Phys. Rev.* B 34 5390
[9] von der Linden W and Horsch P 1988 *Phys. Rev.* B 37 8351
[10] Gygi F and Baldereschi A 1989 *Phys. Rev. Lett.* 62 2160
[11] von der Linden W, Horsch P and Lukas W-D 1986 *Solid State Commun.* 59 485
[12] Ceperley D and Alder B J 1980 *Phys. Rev. Lett.* 45 566
[13] Bachelet G B, Hamann D R and Schlüter M 1982 *Phys. Rev.* B 26 4199
[14] Baldereschi A 1973 *Phys. Rev.* B 7 5212
  Chadi D J and Cohen M L 1973 *Phys. Rev.* B 7 5747
[15] Nelder J A and Mead R 1965 *Comput. J.* 7 308
  Press W H, Flannery B P, Teukolsky S A and Vetterling W T 1986 *Numerical Recipes: the Art of Scientific Computing* (Cambridge University Press: Cambridge) ch 10, p 289
[16] An accurate analysis of the experimental data and of their respective errors is quite important in this context. Data are taken from
  Landolt–Börnstein New Series 1982 Group III, vols 17a, 22a (New York: Springer)
  Aspnes D E and Studna A A 1973 *Phys. Rev.* B 7 4605
  Aspnes D E 1976 *Phys. Rev.* B 14 5331
  Aspnes D E, Olson C G and Linch D W 1976 *Phys. Rev. Lett.* 37 5331
  Straub D, Sibowski M and Himpsel F J 1985 *Phys. Rev.* B 32 5237
  for GaAs, from
  Onton A 1970 *Proc. 10th Int. Conf. on Physics of Semiconductors, Boston (Cambridge, MA, 1970)*
  Monemar B 1973 *Phys. Rev.* B 8 5771
  Guzzi M and Staehli J L 1989 *Physics of the DX Centre in III–V Ternary Compounds* ed J C Bourgoin (Aedermannsdorf: Trans Tech)
  for AlAs, and from
  Hybertsen M S and Louie S G 1986 *Phys. Rev.* B 34 5390
  and references therein, for Ge
[17] Troullier N and Martins J L 1990 *Solid State Commun.* 74 613; 1991 *Phys. Rev.* B 43 1993, 8861
[18] The all-electron calculations referred to in figure 1 are from
  Continenza A, Massidda S and Freeman A J 1988 *Phys. Rev.* B 38 12996
  for ZnSe (FLAPW), from
  Catellani A, Posternak M and Baldereschi A 1992 unpublished
  for ZnO (FLAPW), from
  Catellani A, Posternak M, Baldereschi A and Freeman A J 1987 *Phys. Rev.* B 36 6105
  for BN (FLAPW), from
  Martins J L, Troullier N and Wei S-H 1991 *Phys. Rev.* B 43 2213
  for ZnS (LAPW), from
  Massidda S, Continenza A, Freeman A J, De Pascale T M, Meloni F and Serra M 1990 *Phys. Rev.* B 41 12079

for InP (FLAPW), and from
Carlsson A 1985 *Phys. Rev.* B 31 5178
for Ar, Kr, LiF, NaCl, MgO (ASW). For LiCl, the pseudopotential calculation was by
Hybertsen M S and Louie S G 1986 *Phys. Rev.* B 34 5390
while the dielectric constants are taken from [16] and from
Böer K W 1990 *Survey of Semiconductor Physics* (New York: Van Nostrand-Reynold)

[19]   Fiorentini V and Baldereschi A 1992 *Solid State Commun.* submitted
[20]   Hanke W and Sham L J 1988 *Phys. Rev.* B 38 3361
[21]   Bechsted F and Del Sole R 1988 *Phys. Rev.* B 38 7710
[22]   Resta R 1977 *Phys. Rev.* B 16 2717
[23]   Resta R and Kunc K 1986 *Phys. Rev.* B 34 7146
[24]   Cappellini G, Del Sole R and Reining L 1992 unpublished
[25]   An often-quoted experimental value for AlAs is $m_e^* = 0.15$, given by
Adachi S 1985 *J. Appl. Phys.* 58 R1
This is in fact not an experimental value, being taken from
Casey H C and Panish M B 1978 *Heterostructure Lasers* (New York: Academic)
who in turn make reference to the OPW calculation by
Stukel D J and Euwema R N 1969 *Phys. Rev.* 188 1193
The value used here is from
Dumke W P, Lorenz M R and Pettit G D 1972 *Phys. Rev.* B 5 2978
[26]   de Gironcoli S and Baroni S 1992 unpublished