Spectral properties of quasiparticles in a semiconductor

A. Fleszar and W. Hanke
Institut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany
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The one-electron excitation spectrum of the prototype semiconductor Si has been obtained from a first-principles calculation of the spectral-weight function $A(\vec{q},\omega)$ of the *interacting* one-electron Green's function. The Dyson equation has been solved with the self-energy operator obtained in the GW approximation, where the bare propagator G and the ω-dependent screening matrix W, without (random-phase approximation) and with (time-dependent local density approximation) vertex corrections, have been computed within Kohn-Sham–local-density-approximation theory. Positions of quasiparticle peaks (i.e., the ''band structure''), their lifetimes, and satellite (plasmaron) spectral structures are extracted in a broad energy range. [S0163-1829(97)08140-X]

The momentum- and frequency-dependent spectral-weight function $A(\vec{q},\omega)$ for single-electron excitations is, at least ideally, what is measured by a direct or inverse angular-resolved photoemission experiment in solids: assuming the final states of the emitted photoelectrons are plane waves (an assumption controlled by the energy of the applied photon), neglecting the electron-phonon coupling and extracting from experimental results extrinsic effects (energy losses of the electron on its way to and through the surface) the remaining *primary* photoemission spectrum could be directly interpreted in terms of the spectral function $A(\vec{q},\omega)$ for single-electron excitations. The $\vec{k}$ dispersion of well-defined although broadened (via lifetime effects) quasiparticle peaks gives the *band structure* of a solid. In addition, the function $A(\vec{q},\omega)$ contains other peaks of (usually) smaller spectral weight than the quasiparticle peaks, called the satellites. These structures are also seen in photoemission (PE) experiments.[1]

In this paper we present first-principles results for the spectral-weight function obtained within the lowest-order approximation in the expansion of the self-energy $\Sigma_{\rm xc}$ in the screened Coulomb potential W, i.e., the GW approximation,[2] for the prototypical semiconductor Si. The motivation comes both from experiment and theory: on the one hand, the feasibility of such calculations should have an impact on photoemission experiments, motivating the angular-resolved determination of line shapes and detailed structures (lifetimes, stellites) of the quasiparticle spectrum. On the other hand, first-principles calculations of various physical quantities, for which the *interacting* one-particle Green's function is an input, such as precise extraction of two-particle (optical, etc.) excitations, require the knowledge of both real and imaginary parts of the self-energy and, therefore, of $A(\vec{q},\omega)$.

The dynamics of $N\rightarrow N\pm 1$ excitations, where N is the number of electrons in a solid, is described by the one-electron Green's function $G(\mathbf{r},\mathbf{r}';E)$, which can be obtained from the solution of the Dyson equation:[2]

$$\left(E-\frac{\vec{\nabla}_r^2}{2m}-V_{\rm ext}(\mathbf{r})-V_H(\mathbf{r})-\int d^3r'\Sigma_{\rm xc}(\mathbf{r},\mathbf{r}';E)\right)G(\mathbf{r},\mathbf{r}';E)=\delta(\mathbf{r}-\mathbf{r}'). \tag{1}$$

This equation has a form similar to the Kohn-Sham equations of the density-functional theory,[3] provided the self-energy $\Sigma_{\rm xc}$ is replaced by the Kohn-Sham exchange-correlation potential $V_{\rm xc}$. However, in contrast with the Kohn-Sham potential $V_{\rm xc}$, the self-energy $\Sigma_{\rm xc}$ is a nonlocal, complex, and energy-dependent operator. Due to the complicated self-consistent dependence of $\Sigma_{\rm xc}$ on G, solving Eq. (1) is a difficult task even for the simplest model systems, e.g., jellium. The self-consistency is provided by a closed set of coupled equations (see, e.g., Ref. 2), which in the simplest approximation that includes dynamical polarization processes (RPA), are decoupled by neglecting the vertex corrections. In this case $\Sigma_{\rm xc}$ can be written

$$\Sigma_{\rm xc}(\mathbf{r},\mathbf{r}';E)=\frac{i}{2\pi}\int d\omega e^{-i\omega\delta}G(\mathbf{r},\mathbf{r}',E-\omega)W(\mathbf{r},\mathbf{r}',\omega), \tag{2}$$

where $W(\mathbf{r},\mathbf{r}',\omega)$ is the dynamically screened Coulomb potential, i.e., $W=\epsilon^{-1}v_c$, with ϵ^{-1} the inverse screening matrix. This is the so-called GW approximation.

Application of the GW approach in the framework of first-principles calculations for real solids still remains a computationally extremely demanding task. Despite the fact that the GW method was applied many times to obtain band structures of various materials,[4–7] the main goal of most these calculations has been to explain the observed differences between the energies of experimental PE peaks and the Kohn-Sham eigenvalues. With a few exceptions,[4,6,8] the energy dependence of the dynamically screened Coulomb potential W has been modeled by one of the plasmon-pole schemes proposed in the literature[5] and only the real part of

the self-energy Σ_{xc} in the energy region close to the Fermi level has been calculated. Some work has included specific forms of the vertex function,[4,9] such as excitonic corrections,[4] or calculated in a simplified manner the second-order terms in the expansion of Σ_{xc} in W.[10]

In this paper, we present new results for the prototypical and most studied semiconductor, silicon. We calculate not only the quasiparticle shifts, but rather the full energy dependence of the quasiparticle spectral-weight function $A(\mathbf{r},\mathbf{r}';\omega)$, which is defined by the equation

$$G(\mathbf{r},\mathbf{r}';\omega)=\int_{-\infty}^{\infty}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{\omega-\omega'}d\omega', \tag{3}$$

where $G(\mathbf{r},\mathbf{r}';\omega)$ is the *interacting* Green's function. The spectral-weight function $A(\omega)$ contains experimentally accessible informations through the energy position and width of the main quasiparticle peak. The additional structures (satellites) also belong to the experimentally observed spectrum.[1]

General properties of quasiparticle spectral-weight functions in silicon and diamond have been recently studied in a model calculation by Bechstedt *et al.*[11] Also recently, Rojas, Godby, and Needs[12] proposed a ''real-space/imaginary-time'' scheme of calculating the self-energy in solids. From the self-energy obtained at the *imaginary-energy axis* they derive the spectral-weight function of silicon at the *real-energy axis* via an extrapolation procedure. Here we do not use this method, but instead calculate the self-energy directly on the real-ω axis and project the screened Coulomb interaction W into reciprocal space. The self-energy operator is obtained in the GW approximation, with the bare propagator G and the dynamically screened Coulomb potential W, without [in random-phase approximation (RPA)] and with vertex corrections [in time-dependent LDA (TDLDA)], being computed within Kohn-Sham theory in the local-density approximation (LDA). The self-energy and the function $A(\vec{k},\omega)$ are calculated for a number of $\vec{k}$ vectors across the Brillouin Zone (BZ). In this way, a plot of the ''band structure'' in silicon in terms of the dispersion of the spectral-weight function is obtained. In addition, we extract the energy dependence of many-body shifts and quasiparticle inverse lifetimes for states ranging up to 70 eV above the Fermi level. Our results indicate that the simple model of a constant shift of quasiparticle bands with respect to the Kohn-Sham bands (the *scissor operator*) becomes inadequate beyond a few eV range from the Fermi level and that beyond this energy range, the behavior of the quasiparticle self-energy shifts and of the inverse lifetime resembles qualitative features of the behavior of these quantities in the jellium model.[2,13]

Using in Eq. (2) the noninteracting Green's function, expressed in terms of Kohn-Sham–LDA orbitals ψ_{kn} and energies ε_{kn} (the subscripts ''k'' and ''n'' denote the wave vector $\vec{k}$ and the band index n, respectively), one has the following expression for the correlation part of Σ_{xc} (the remaining part is the pure exchange self-energy):

$$\Sigma_c(\mathbf{r},\mathbf{r}';E)=\sum_{kn}\psi_{kn}(\mathbf{r})\psi_{kn}^*(\mathbf{r}')\Bigg[\widetilde{W}(\mathbf{r},\mathbf{r}';\varepsilon_{kn}-E)\times[\theta(E-\varepsilon_{kn})-\theta(\varepsilon_F-\varepsilon_{kn})]-\frac{1}{\pi}\int_0^{\infty}d\omega\frac{E-\varepsilon_{kn}}{(E-\varepsilon_{kn})^2+\omega^2}\widetilde{W}(\mathbf{r},\mathbf{r}';i\omega)\Bigg], \tag{4}$$

where ε_F is the Fermi energy and $\widetilde{W}=W-v_c$, with v_c the Coulomb interaction. We have evaluated expression (4) in the space spanned by the Bloch functions of the corresponding LDA Kohn-Sham Hamiltonian using the exchange-correlation potential of Ceperley and Alder.[14] The interaction with the ionic cores was replaced by the non-local pseudopotential as in Ref. 15. A plane-wave basis set was used to solve for the LDA Bloch functions. The applied cutoff of 18 Ry corresponds to $\sim$340 plane waves and describes well the occupied and the unoccupied states in the excited-energy range relevant for Eq. (4). The ω-dependent inverse dielectric matrix ϵ^{-1}, necessary to build up the W operator, was calculated at the uniform mesh of $\vec{k}$ points in the BZ from the LDA bands.[16] No plasmon-pole approximation was applied. Instead, the screening matrix was calculated at the discrete mesh of energies ranging from 0 to 100 eV with a step of 0.5 eV. An interpolation between energy-mesh points to the actual energy argument $\varepsilon_{kn}-E$ was applied for each matrix element of the operator $\widetilde{W}$. The integral over energies on the right-hand side of Eq. (4), where the screening operator is taken along the imaginary-energy axis, was performed by a Gaussian quadrature. We note in passing that Σ_c converges rather slowly with the number of bands n in Eq. (4). Here we use 100 (conduction) bands and find that taking only 50 bands results in an upwards shift of $\sim$0.2 eV in the energy position of the topmost occupied state at $q=0$. This is an important point, as the energy position of the topmost occupied state determines various physical observables, such as the ionization potential, work function at the surface of the solid, or the band offset at the interface. Interestingly, the value we obtain for the energy position of the topmost occupied quasiparticle peak at the Γ point is about 0.2 eV lower than all previously published results known to us. We think this discrepancy is caused by the above mentioned slow convergence in Σ_c.

In Fig. 1 the dispersion of the spectral-weight function $A(\vec{k},\omega)$ for $\vec{k}$ along L-Γ-X directions is shown. The quantity displayed is Tr $A(\vec{k},\omega)$, where the trace is taken in the subspace of Bloch functions with fixed wave vector $\vec{k}$. The zero point of the energy is at the energy of the topmost occupied LDA–Kohn-Sham eigenvalue. There is an energy region around the absolute gap for which the quasiparticle peaks in the GW approximation become a renormalized δ function $Z_k\delta(\omega-E_k)$, with $Z_k=(1-\partial\Sigma/\partial\omega)^{-1}$. The imaginary part of the self-energy is then strictly zero due to the absence of electron-hole excitations, which can absorb the energy of a decaying quasiparticle. The size of this region is given by the smallest possible excitation energy contained in $W(E)$, which is equal to the absolute gap (in our case the LDA gap), if one assumes the RPA in screening, i.e., no excitonic effects.[4] Since the LDA gap is much smaller than the

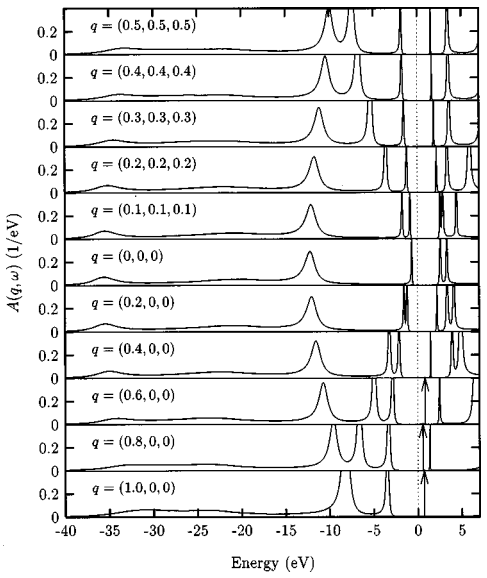

FIG. 1. The spectral-weight function for quasiparticles in Si along L-Γ-X directions calculated within the RPA approximation. The $\vec{q}$ vector is given in units of $2\pi/a$, where $a=10.261$ a.u. The energy zero is fixed at the energy of the topmost occupied LDA state at the Γ point. Arrows indicate quasiparticle peaks, which are renormalized δ functions.

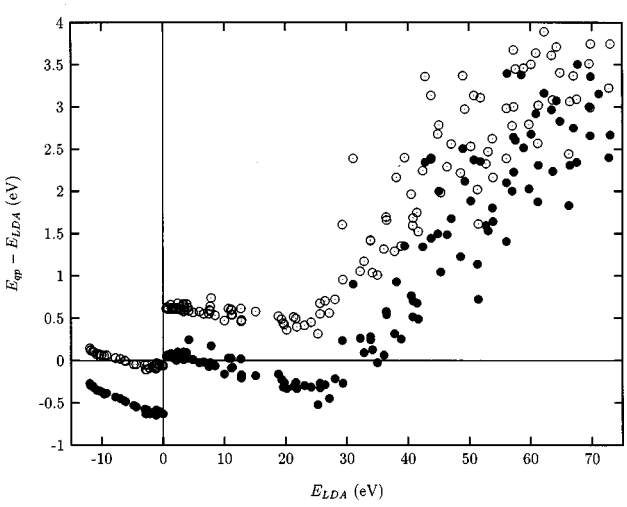

FIG. 2. The shift of quasiparticle energies $E_{\rm qp}-E_{\rm LDA}$ as a function of the corresponding Kohn-Sham–LDA energy $E_{\rm LDA}$. $E_{\rm qp}$ is the energy position of the quasiparticle peak. Full circles are the result of the standard (RPA) GW calculation [Eq. (2)], the empty circles have the TDLDA vertex function included. The shifts were calculated along the L-Γ-X lines.

''true,'' or ''GW'' gap, we obtain a nonzero width for quasiparticle peaks close to the topmost occupied state, which should be δ-function-like peaks in a fully self-consistent GW calculation. For example, the energy shift with respect to the LDA value for the topmost occupied state is -0.63 eV, which therefore falls below the LDA electron-hole excitation threshold (Auger treshold), which is 0.51 eV. A self-consistency cycle in the calculation of the GW self-energy would restore the δ-like shape for this and other states within the Auger threshold. One should remember, however, that for states near the Fermi level the width of experimental peaks must be much larger than the GW theory can predict. One (technical) reason is the fact that experiments are always done with a certain instrumental accuracy, which contributes to the width of measured peaks. Another (physical) reason is the fact that close to the Fermi level other mechanisms not included in the purely electronic and perfectly periodic bulk Hamiltonian, such as scattering on crystal imperfections or interaction with phonons, could be more efficient in broadening the quasiparticle linewidth. We expect, however, that beyond a few eV above and below the Fermi level, i.e., in the energy region where the electron-electron interaction is a dominant relaxation mechanism, our predictions are quantitatively correct. An interesting many-body feature of the quasiparticle spectral lines is the presence of plasmon satellites. They are clearly seen in Fig. 1 as broad peaks below the lowest occupied quasiparticle band. In our calculation the energy position of the satellite peaks comes out to be about 1.5 of the plasmon energy below a given quasiparticle peak. This seems to be an overestimation of the binding energies of plasmon satellites and a feature of the GW approximation. Experimentally, at least for core spectra and some available valence spectra of simple metals, plasmon satellites are shifted by the plasmon energy.[1] Ways of correcting for this overestimation have been proposed, which go beyond the GW approximation.[17] Unfortunately, to the best of our knowledge, angular-resolved photoemission experiments in the valence-band region of silicon do not extend thus far below the Fermi energy. We hope to motivate with our results new high-resolution experiments focused on the determination of the detailed fine structures of the quasiparticle spectrum: the plasmon satellites and the line shapes.

Full circles in Fig. 2 display the many-body shifts of quasiparticle energies as a function of the corresponding LDA single-particle energies, calculated for states along the L-Γ-X lines. The shifts were obtained from the positions of peaks in the spectral functions projected onto each Bloch state.[18] A few important points should be noted. First, it is seen that beyond a small region of 3–5 eV around the Fermi level the many-body shifts are far from being constant. In particular, a clear dip in the value of shifts is visible for quasiparticle energies between 10 and 30 eV above the Fermi level. Such a dip, which has been obtained also for the self-energy in jellium,[2,13] arises as the result of the enhanced probability of plasmon emission, when the quasiparticle energy is high enough. At and beyond this energy region quasiparticle-energy shifts grow rapidly. There exists a rather large scattering of the shift values for quasiparticle states with similar (LDA) energies. This scattering reflects the spatial behavior of the self-energy in a real material: a projection of $\Sigma_{\rm xc}$ on different Bloch functions with different spatial and symmetry properties gives quite different results.

In contrast to previously published results, almost all of the contribution to the increase of the LDA absolute gap stems in our calculation from the downwards shift of occupied states. While the topmost occupied state is shifted down by 0.63 eV, the lowest unoccupied state moves only up by 0.05 eV. Since the position of the topmost occupied state should be exactly given by the (exact) Kohn-Sham formalism, the question arises as to whether, for silicon, the LDA approximation used in the Kohn-Sham equations strongly overestimates (moves up) the energy of the topmost occu-

TABLE I. The positions of the main quasiparticle peaks in the spectral function in silicon for some states in eV. The energy zero is put at the topmost occupied LDA–Kohn-Sham energy. GW refers to results obtained with Eq. (4), $GW\Gamma$ when vertex corrections were included according to Ref. 9.

	LDA	GW	$GW\Gamma$
Γ_{1v}	−11.93	−12.20	−11.78
$\Gamma_{25'v}$	0.00	−0.63	−0.06
Γ_{15c}	2.55	2.60	3.16
$\Gamma_{2'c}$	3.26	3.33	3.93
X_{1v}	−7.77	−8.20	7.74
X_{4v}	−2.83	−3.46	−2.94
X_{1c}	0.65	0.72	1.28
$L_{2'v}$	−9.58	−9.98	−9.53
L_{1v}	−6.96	−7.41	−6.94
$L_{3'v}$	−1.19	−1.83	−1.28
L_{1c}	1.50	1.55	2.12
L_{3c}	3.33	3.43	3.99
Absolute gap	0.51	1.19	1.19
Occupied-band width	11.93	11.57	11.72

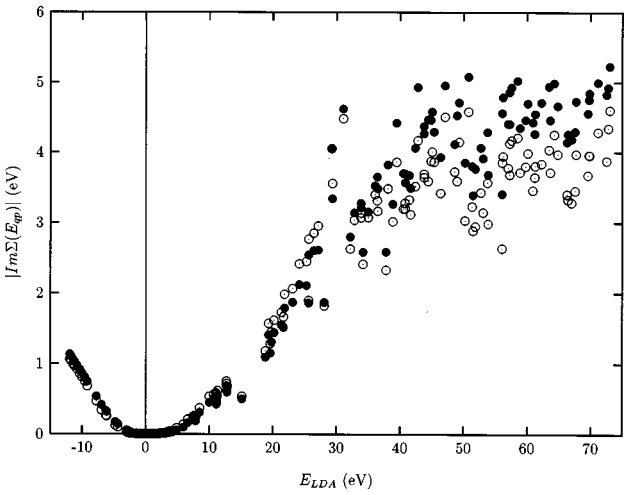

FIG. 3. Diagonal matrix elements of the imaginary part of the self-energy between Kohn-Sham–LDA orbitals, calculated at the energy of the corresponding quasiparticle peak. The full circles are the result of the standard (RPA) GW calculation [Eq. (2)], the empty circles have the TDLDA vertex function included. The self-energy is calculated along the L-Γ-X lines.

pied state, or whether the GW approximation to the full many-body self-energy strongly underestimates (moves down) this energy. The latter possibilty would point to the importance of vertex corrections in the calculation of the self-energy. The fact that the work function in silicon is rather well described within the LDA[19] indicates that the inclusion of vertex corrections is required.

Treating vertex corrections systematically, i.e., respecting conservation laws, is extremely difficult even for the simplest homogeneous electron-gas system. As first shown by Hanke and Sham[20] and later again by Del Sole, Reining, and Godby,[9] taking into account screening with the induced exchange-correlation field within the LDA approximation (the *adiabatic* TDLDA approach[21]) leads to a many-body vertex function, which in effect ''renormalizes'' the screened Coulomb interaction: $W'=[1-\chi^0(v_c+f_{\rm xc})]^{-1}v_c$, with $f_{\rm xc}=\delta V_{\rm xc}^{\rm LDA}/\delta n$.[22] As in Ref. 9, we will call this approach the $GW\Gamma$ approach. The physical interpretation of this picture is appealing: the bare Coulomb interaction of the ''extra'' particle injected into the solid is screened not with the *test charge–test charge* dielectric function, but with the *test charge–electron* dielectric function,[23] although the induced exchange-correlation field is described only approximately. Empty circles in Fig. 2 show many-body shifts obtained in this case. As already noted in Ref. 9, the quasiparticle and LDA energy of the topmost occupied state almost coincide in this case. Table I summarizes some results obtained in this work for quasiparticle energies at various states.

Figure 3 gives the energy dependence of the imaginary part of the self-energy calculated at the quasiparticle energy.[24] The imaginary part of Σ_c originates from the first term in the square bracket in Eq. (4) [$\tilde{W}(\mathbf{r},\mathbf{r}';i\omega)$ in the second term in Eq. (4) is real], This term provides a clear physical interpretation for the lifetime of a quasiparticle: the presence of the difference of the two-step functions in Eq. (4) allows the quasiparticle to decay to those *empty* states only, whose energy is between the quasiparticle energy and the Fermi level (in the case of a hole the empty state means a state occupied by an electron). Energy and momentum released in the transition are absorbed by excitations of the system present in Im($\tilde{W}$), which is connected to the *loss function*. It is interesting to note that the overall shape of both plots in Fig. 2 and Fig. 3 is quite similar to corresponding plots for the case of jellium.[2,13] Apart from the lack of full rotational symmetry in a real solid and the effects of the crystal potential, which give rise to a certain scattering of results for states close in energy, and apart from the obvious differences in the behavior of the real and imaginary parts of self-energy in the energy region around the Fermi level,[25] the similarity is rather striking. In particular, as in the case of jellium, the imaginary part of the self-energy reaches a kind of a ''saturation'' region for quasiparticle energies high enough to decay with the emission of a plasmon. As in Fig. 2, the full circles in Fig. 3 show results obtained with the standard (RPA) GW approximation, while empty circles refer to the case in which the vertex function is included within the TDLDA theory. While inclusion of the vertex corrections decreases the value of the imaginary part of the self-energy for quasiholes, it increases it for quasielectrons in the energy region up to $\sim$30 eV above the Fermi level. This was to be expected: within the adiabatic TDLDA approach the *real* factor $f_{\rm xc}$ in W' leaves the imaginary part of W' almost unaffected for small energies, but contributes to the increase of the real part. As a consequence, the positions of quasiparticle peaks are shifted by about 0.6 eV to higher energies, as seen in Fig. 2. This means that they are shifted to the region of smaller Im Σ for occupied states and to larger ImΣ for unoccupied states. For quasiparticle energies higher than 30 eV there is already a pronounced difference in the imaginary part of self-energy when $f_{\rm xc}$ is included in the screening. The net effect is to increase the quasiparticle lifetime in this energy region.[26]

In conclusion, we have presented the ''band structure'' of a real solid in terms of the spectral-weight function, with an

ab initio account of electron-ion and electron-electron interactions. Plots, as shown in Fig. 1 for silicon, correspond to what is usually called the *primary* photoemission spectrum and should prove useful for the detailed analysis of photoemission measurements. The feasibility of first-principles calculations of the spectral-weight functions $A(\vec{q},\omega)$ should have an impact on direct and inverse PE experiments and motivate new, high-resolution measurements focused on the determination of detailed spectral features, quasiparticle lifetimes, and the satellite structures. In accordance with general expectations it was demonstrated that, beyond a small region of a few eV around the Fermi level, the energy dependence of the quasiparticle shifts and of the widths of spectral peaks very much resemble the jellium results. The often used concept of the ''scissor operator'' becomes particularly inaccurate there and the quasiparticle shifts have rather strong energy dependences. Our calculation of the energy dependence of the lifetime due to electron-electron interactions is, to our knowledge, the first such calculation with fully *ab initio* methods for a real solid.[27] This result shows that the commonly used empirical optical potential can be replaced by a fully *ab initio* calculation of the self-energy.

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[24] We could have displayed alternatively the full width of the spectral peaks, which is a quantity roughly twice as big. We prefer to show the imaginary part of the self-energy because of the direct connection of this quantity with the empirical optical potential commonly used in various calculations.

[25] In contrast with the case of a metal, for an insulator there is a jump in the quasiparticle shifts across the Fermi level. The imaginary part of self energy starts to be nonzero only beyond the ''Auger gap,'' which in our case is determined by the LDA gap.

[26] Another way of understanding the effect of vertex corrections on the quasielectron lifetime could be the following: it is known that vertex corrections generally shift the spectral intensity of excitations in the system (loss properties) into the region of lower energies. Therefore, for energies lower than the energy of the main loss peak, the absolute value of ImW' should be greater than the absolute value of ImW, while for energies bigger, it is the opposite.

[27] Similar calculations, based however on a more simplified description of the *unperturbed* band structure, have been presented by one of us (W.H.) in Ref. 4.