The charge density of semiconductors in the GW approximation

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We present a method to calculate the electronic charge density of periodic solids in the GW approximation, using the space-time method. We investigate for the examples of silicon and germanium to what extent the GW approximation is charge-conserving and how the charge density compares with experimental values. We find that the GW charge density is close to experiment and charge is practically conserved. We also discuss how using a Hartree potential consistent with the level of approximation affects the quasi-particle energies and find that the common simplification of using the LDA Hartree potential is a very well justified.

I. INTRODUCTION

Amongst the established methods to calculate the electronic properties of solids, Hedin's GW approximation[1] is notable for its unrivalled success in predicting the energy gaps of semiconductors and insulators (e.g. Refs. 2–5). Unlike alternative methods which are based on density functional theory and describe ground state properties by mapping the many-electron problem onto an effective one-electron problem, it seeks to find a solution for the exact one-particle Green's function of the many-electron system to which it is applied. With this knowledge, a wide range of properties of the system under consideration can be accurately described, among them the optical excitation spectrum, the density of states, the charge density and the total energy.

As an exact solution of the many-electron problem remains today as elusive as ever, any attempt to determine the Green's function has to rely on skilled approximations. The problem of finding the exact Green's function of a system is equivalent to finding its self-energy. In the GW approximation, this quantity is approximated by the product of G, the Green's function, and W, the screened Coulomb interaction; hence the name.

GW calculations for semiconductors so far have concentrated on the optical excitation spectrum, the one area where GW has had its most striking successes, but other aspects of electronic structure have not been investigated with this method for real materials. This is largely due to the prohibitively large numerical effort. Recently, however, a new technique has been developed, the GW space-time method,[6] that makes GW calculations much faster and allows a precise computation of the energy dependence of the self-energy without recourse to plasmon pole models. This opens up the way to new applications for the GW formalism.

In this paper we will concentrate on the electronic charge density[7] of semiconductors, present a new technique for extracting it from the Green's function at GW level and show for the first time results of GW charge density calculations for real materials at the example of Si and Ge, for which very careful analyses of the experimental data are available for comparison.[8,9] We also investigate the problem of charge conservation and the influence of using a Hartree potential consistent with the level of approximation on the quasi-particle spectrum.

Atomic units are used throughout unless otherwise noted.

II. THEORY

The central equation of the GW approximation is the expression for the self-energy:

$$\Sigma(\mathbf{r},\mathbf{r}';\tau) = iG(\mathbf{r},\mathbf{r}';\tau)W(\mathbf{r},\mathbf{r}';\tau). \tag{2.1}$$

Full self-consistency in the GW approximation would mean that the Green's function that enters into Eq. (2.1) were itself a solution of the equation

$$\left(-\frac{1}{2}\nabla^2 + V_{ext}(\mathbf{r}) + V_H^{SC}(\mathbf{r}) + \Sigma^{SC}(\mathbf{r},\mathbf{r}';\omega)\right) G(\mathbf{r},\mathbf{r}',\omega) = -i\delta(\mathbf{r},\mathbf{r}') \tag{2.2}$$

where the superscript SC for Σ and the Hartree potential V_H indicates that these quantities have been determined self-consistently. In the case of the Hartree potential this means the charge density at GW level has to be known. Such a self-consistent GW calculation has never been done for a real system and there are indications[10] that self-consistency will destroy the good agreement between the computed and experimental quasi-particle spectrum.

In this paper we employ the usual one-iteration non-self-consistent GW approximation. However, we will determine the charge density and thus the Hartree potential self-consistently at a level where the self-energy is kept fixed at its first-iteration value. The charge density itself is an indicator as to whether such an approach is justified, as it has been shown by Baym and Kadanoff[11,12] that generally only self-consistent approximations to the self-energy conserve particle number strictly. We will therefore monitor carefully whether our approach violates particle number.

The traditional way to set up and solve the GW equations has been to express and compute all quantities in the reciprocal space and energy domain. This involves sums scaling with the fourth power of the number of plane waves N used to represent the wavefunctions. Rojas, Godby and Needs[6] have shown recently that using the most appropriate representation at the various stages of the computation, either real space and time or reciprocal space and energy, and changing between representations by means of Fast Fourier Transforms, can bring this scaling down to N^2, thus leading to very significant time savings.

Another point noted by Rojas et al. is that a detailed calculation of all relevant quantities along the imaginary time or imaginary energy axis is possible without recourse to a plasmon pole or similar model. This is because on the imaginary time axis the Green's function, the polarisability and the self-energy are all rapidly decaying smooth functions which can easily be represented on a regular grid. Transformation to imaginary energy via an FFT is straightforward. If the properties of Σ on the real energy axis are needed, analytic continuation with the help of model functions is possible. However, for the calculation of the charge density alone, the knowledge of the self-energy on the imaginary energy axis only is sufficient.

Having determined the self-energy Σ on the imaginary energy axis as described in Ref. 6, with

$$\Sigma(\mathbf{r},\mathbf{r}';i\tau) = iG_0(\mathbf{r},\mathbf{r}';i\tau)W(\mathbf{r},\mathbf{r}';i\tau), \tag{2.3}$$

where G_0 is the Green's function at LDA level, the Green's function G at GW level obeys the Dyson equation

$$\begin{aligned} G(i\omega) = G_0(i\omega) + G_0(i\omega) \times \\ \times \left(\Sigma(i\omega) + \Delta V_H - V_{xc} - \epsilon_0\right) G(i\omega) \end{aligned} \tag{2.4}$$

where G, G_0, Σ, ΔV_H and V_{xc} in this notation are to be understood as matrices in a plane-wave basis and matrix multiplication of the factors on the right hand side is implied. ΔV_H is the change in the Hartree potential due to the density change and has to be determined self-consistently, V_{xc} is the LDA exchange correlation potential and ϵ_0 represents the shift in the Fermi level with respect to the vacuum in the GW calculation from its value in the LDA. The use of this shift ϵ_0 was first proposed by Hedin[1] but is often neglected in GW calculations. We use it here to introduce an element of self-consistency into the equations by ensuring that the Fermi energy is the same before and after applying the GW correction. Eq. (2.4) can directly be solved by matrix inversion.

The relationship between charge density ρ and Green's function is given by the equation

$$\rho(\mathbf{r}) = -\frac{2}{\pi}\int_{-\infty}^{0} d\omega \mathrm{Im}G(\mathbf{r},\mathbf{r};\omega) \tag{2.5}$$

where it is assumed that the zero of energy is chosen at the Fermi level.

Since we know the charge density at the LDA level of approximation we only need to evaluate the charge density difference $\Delta\rho$ between the LDA and the GW result. The Green's function has poles in the second and fourth quadrant of the imaginary plane, just infinitesimally off the real axis. Using Cauchy's Theorem and the fact that for complex energy z $\Delta G(z)$ vanishes quadratically as $|z| \to \infty$, where $\Delta G = G - G_0$, we know that the charge density difference can just as well be calculated by an integration along the imaginary energy axis:

$$\Delta\rho(\mathbf{r}) = -\frac{2}{\pi}\int_{-\infty}^{0} d\omega \mathrm{Re}\Delta G(\mathbf{r},\mathbf{r};i\omega). \tag{2.6}$$

This means that the knowledge of the Green's function along the imaginary axis is sufficient to calculate the charge density at GW level without the need for explicit analytic continuation to the real energy axis, which would inevitably have to involve some sort of model.

In theory, the integration of $\Delta G(i\omega)$ according to Eq. (2.6) is straightforward. In practice, in order to achieve satisfactory convergence in a numerical integration, one would have to include such a large number of energy points in the integration, as to make it prohibitively expensive, because for each energy point the self-energy would first have to be computed and the Dyson equation solved. On the other hand, we know that the self-energy as a function of imaginary energy decays quadratically for large energies. This allows us for large ω to make an expansion of $G(i\omega)$ in powers of $1/\omega$ and neglect terms of order higher than $1/\omega^2$. The perturbatively treated high-energy tail can be integrated analytically from some energy ω_0 to infinity, as we will show in the appendix. Up to ω_0 we integrate Eq. (2.6) numerically. ω_0 is thus treated as a convergence parameter.

For each new $\Delta\rho$ we compute a new ΔV_H and solve Eqs. (2.4) and (2.6) repeatedly until ΔV_H is stable.

III. RESULTS

Before we can make comparisons to experimental results we have to account for the fact that we work in the pseudopotential approximation. This means that the charge density computed as described in the previous section contains no contribution from the core electrons and the contribution of the valence electrons is modified in the core region as well.

We follow Nielsen and Martin[13] in writing the total charge density as the superposition of the atomic densities plus a deformation density ρ_{def}, which is defined in reciprocal space as

$$\rho_{\mathrm{def}}(\mathbf{G}) = \rho_{\mathrm{solid,ps}}(\mathbf{G}) - S(\mathbf{G})\rho_{\mathrm{atom,ps}}(\mathbf{G}), \tag{3.1}$$

where $\mathbf{G}$ is a reciprocal lattice vector, S the structure factor of the crystal and $\rho_{\mathrm{solid,ps}}$ the charge density generated by the pseudowavefunctions of the valence electrons in the solid and $\rho_{\mathrm{atom,ps}}$ the same in the free atom.

The Fourier coefficients of the total charge density in the solid are then computed according to

$$\rho_{\rm solid}(\mathbf{G}) = S(\mathbf{G})\rho_{\rm atom}(\mathbf{G}) + \rho_{\rm def}(\mathbf{G}), \qquad (3.2)$$

where $\rho_{\rm atom}$ is the full charge density of valence and core electrons of a free atom. This approach assumes rigid cores, in line with the assumptions underlying the pseudopotential method.

Where we find that the charge in the *GW* approximation is not strictly conserved, we normalise the density by multiplying all structure factors computed according to Eq. (3.2) by a constant that assures the overall correct number of electrons per unit cell.

The results we present in this section come from LDA calculations that were performed with pseudopotentials generated by the Hamann method,[14] a plane-wave cutoff of 17Ry for Si and 20Ry for Ge and 10 special **k** points. For Ge relativistic effects were included in the pseudopotential but no spin-orbit coupling was taken into account in the solid. A Ceperley-Alder exchange correlation potential[15] was used in the parametrisation by Perdew and Zunger.[16] In the *GW* space-time calculation we used 65 bands truncated to 169 plane waves from the LDA calculation. The time grid comprised 60 points spaced at 0.314 a.u. which were zero-padded to 120 points before transformation to imaginary energy, giving an ω_0 of 10 Hartrees. Other parameters of the *GW* calculation were as described in Ref. 6.

Table I shows our computed structure factors of the pseudo valence charge of silicon for several reciprocal lattice vectors **G**. The second column shows the LDA values and the third the *GW* correction $\Delta\rho$. $\Delta\rho$ is actually the difference between the normalised *GW* density and the LDA density. Without normalisation the *GW* valence density integrates to a total of 8.0233 electrons per unit cell (instead of 8), a charge violation of not quite 0.3%. This observation of a very small but finite charge violation is in line with rigorous analytical results by Schindlmayr for a model system.[17] The fourth column lists the (normalised) *GW* correction to the density that results if the Hartree potential is kept fixed at its LDA value. As one would expect, this unscreened correction is larger. However, because contributions from all energies are integrated over and we are looking at non-zero **G** the screening effect is much weaker than one might naively expect by scaling down with the dielectric constant. The LDA structure factors of the pseudo valence charge are themselves not very meaningful, as they depend to some extent on the specific pseudopotential used. They are only listed to give an idea of the relative magnitude of the *GW* correction.

Table II shows the structure factors of the total density of Si for several reciprocal lattice vectors. The second column lists the LDA values and the third the (normalised) *GW* values. The biggest contribution comes actually from the cores, as the comparison with the valence structure factors in Table I shows, so that now the difference between the LDA and the *GW* structure factors looks even less significant. Because of the weight of the core contribution the lattice constant has a crucial influence on the structure factors. We have used for both the LDA and the *GW* calculation the experimental value of 5.43Å. In the last column we list experimental static (zero temperature) structure factors for comparison. They are the Fourier transforms of a model fit[18,8] to experimental data. The agreement of both *GW* and LDA with experiment is very good.

Table III gives the valence structure factors of germanium and the *GW* correction to it. The raw *GW* valence density integrates to 8.004 electrons per unit cell (instead of 8), a charge violation of 0.05%. The values shown are for the normalised density and values for the unscreened correction are given as in Si. Table IV compares the full LDA and *GW* density structure factors in bulk Ge with experimental static structure factors from Ref. 9 (fit C in their Table III). The agreement of both LDA and *GW* values with experiment is again very good. We have used a Ge lattice constant of 5.66Å in LDA and *GW* calculations.

Note that the structure factors listed in the tables have to be multiplied by the diamond lattice structure factors $S(\mathbf{G})$ to get the Fourier coefficients of the charge density in the crystal as expressed by Eq. (3.2).

Small though the differences between the LDA and *GW* densities are, we can see that for both Si and Ge the *GW* charge in real space is slightly less concentrated near the atom sites and moves a little into the interstitial and bonding regions. As a trend this goes into the right direction since it is known that the LDA tends to accumulate too much charge near the atoms. Figs. 1 and 2 show the charge density differences in Si and Ge along the edge of a conventional cell between two atom sites.

We give a list of quasiparticle energies at several symmetry points for Si in Table V and for Ge in Table VI. The second column gives the values with the Hartree potential taken at LDA level and the third with a Hartree potential which uses the *GW* density. One can see that the influence of ΔV_H on the quasi-particle energies is very small.

IV. CONCLUSION

The results presented in the previous section show that in the materials we have investigated the *GW* approximation can for most practical purposes be considered to be charge conserving. It could be demonstrated that the charge density is very close to experimental values and also little different from the density at LDA level. This gives support to the common practice of computing the quasi-particle corrections to the LDA eigenvalues without adjusting the Hartree potential. Adjusting the Hartree potential to the *GW* density has only a small effect on the quasi-particle energies.

V. APPENDIX

To show how we treat the high-energy tail of the integrand in Eq. (2.6) let us rewrite Eq. (2.4) in the form

$$G(i\omega) = F^{-1}(i\omega)G_0(i\omega), \tag{5.1}$$

$$F(i\omega) = \big(1 - G_0(i\omega)\left[\Sigma_{xc}(i\omega) + \Delta V_H - V_{xc} - \epsilon_0\right]\big). \tag{5.2}$$

For large ω, as G_0 decays as $1/\omega$, we can expand F^{-1} in powers of G_0, keeping in mind that Σ itself contains one factor G_0. To first order in G_0 then

$$\lim_{\omega\to-\infty} F^{-1}(i\omega) = 1 + G_0(i\omega)\left[\Sigma_x + \Delta V_H - V_{xc} - \epsilon_0\right], \tag{5.3}$$

where Σ_x is the exchange part of the self-energy that does not itself depend on the high energy tail of G_0,

$$\Sigma_x(i\omega) = G_0(0)V_c, \tag{5.4}$$

where V_c denotes the inter-electronic Coulomb interaction.

To this order of approximation then

$$\begin{aligned}&\lim_{\omega\to\infty} \Delta G(i\omega)\\ &= G_0(i\omega)\left[\Sigma_x + \Delta V_H - V_{xc}\right]G_0(i\omega).\end{aligned} \tag{5.5}$$

After a few transformations we can find from this

$$\begin{aligned}&\lim_{\omega\to-\infty} \mathrm{Re}\Delta G(\mathbf{r},\mathbf{r};i\omega) =\\ &\sum_{\mathbf{k}}\sum_{nn'}\Big\{\mathrm{Re}\left[\Psi_{n\mathbf{k}}(\mathbf{r})\Psi_{n'\mathbf{k}}(\mathbf{r})P_{nn'}(\mathbf{k})\right] f^{(1)}_{nn'}(\omega;\mathbf{k})\\ &-\mathrm{Re}\left[\Psi_{n\mathbf{k}}(\mathbf{r})\Psi_{n'\mathbf{k}}(\mathbf{r})P_{nn'}(\mathbf{k})\right] f^{(2)}_{nn'}(\omega;\mathbf{k})\Big\}\end{aligned} \tag{5.6}$$

where

$$f^{(1)}_{nn'}(\omega;\mathbf{k}) = \mathrm{Re}\frac{1}{(\omega_{n\mathbf{k}} - i\omega)(\omega_{n'\mathbf{k}} - i\omega)}, \tag{5.7}$$

$$f^{(2)}_{nn'}(\omega;\mathbf{k}) = \mathrm{Im}\frac{1}{(\omega_{n\mathbf{k}} - i\omega)(\omega_{n'\mathbf{k}} - i\omega)}, \tag{5.8}$$

$$\begin{aligned}P_{nn'}(\mathbf{k}) = &\sum_{\mathbf{G},\mathbf{G}'}\Psi_{n\mathbf{k}}(\mathbf{G})\left[\Sigma_x(\mathbf{k},\mathbf{G},\mathbf{G}')\right.\\ &\left.+\Delta V_H(\mathbf{G}-\mathbf{G}') - V_{xc}(\mathbf{G}-\mathbf{G}')\right]\Psi_{n'\mathbf{k}}(\mathbf{G}').\end{aligned} \tag{5.9}$$

The advantage of this formulation is that the energy dependent parts can be integrated analytically. We therefore split up the integration in Eq. (2.6) into two parts, the first of which is performed numerically up to some suitably chosen value ω_0 and the remainder of the integral from ω_0 to $-\infty$ is evaluated analytically by using the relationship

$$\begin{aligned}&\int_{-\infty}^{\omega_0} f^{(1)}_{nn'}(\mathbf{k})(\omega)d\omega\\ &= \begin{cases}\frac{1}{\omega_{n\mathbf{k}}-\omega_{n\mathbf{k}'}}\left[\arctan\frac{\omega_0}{\omega_{n\mathbf{k}'}} - \arctan\frac{\omega_0}{\omega_{n\mathbf{k}}}\right] & \text{if } \omega_{n\mathbf{k}} \neq \omega_{n'\mathbf{k}}\\ \frac{1}{\omega_{n\mathbf{k}}}\frac{\omega_0/\omega_{n\mathbf{k}}}{1+(\omega_0/\omega_{n\mathbf{k}})^2} & \text{if } \omega_{n\mathbf{k}} = \omega_{n'\mathbf{k}}\end{cases}\end{aligned}$$

and

$$\begin{aligned}&\int_{-\infty}^{\omega_0} f^{(2)}_{nn'}(\mathbf{k})(\omega)d\omega\\ &= \begin{cases}\frac{1}{2(\omega^{>2}-\omega^{<2})}\ln\frac{\omega_0^2+\omega_{n\mathbf{k}}^{<2}}{\omega_0^2+\omega_{n\mathbf{k}}^{>2}} & \text{if } \omega_{n\mathbf{k}} \neq \omega_{n'\mathbf{k}}\\ -\frac{1}{2(\omega^{>2}+\omega^{<2})} & \text{if } \omega_{n\mathbf{k}} = \omega_{n'\mathbf{k}}\end{cases},\end{aligned}$$

with $\omega^{<} = \min\left(|\omega_{n\mathbf{k}}|, |\omega_{n\mathbf{k}'}|\right)$, $\omega^{>} = \max\left(|\omega_{n\mathbf{k}}|, |\omega_{n\mathbf{k}'}|\right)$

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TABLE I. Structure factors (absolute values) of the pseudo valence charge density of Si [e/atom] at LDA level and the correction from the GW approximation with and without adjusting the Hartree potential.

G	LDA valence	$\Delta\rho$	$\Delta\rho$

		(V_H GW)	(V_H LDA)
1 1 1	1.2487	-0.0054	-0.0076
2 2 0	0.0323	-0.0035	-0.0043
3 1 1	0.2429	-0.0023	-0.0023
4 0 0	0.1877	0.0009	0.0012
3 3 1	0.0601	0.0021	0.0023
4 2 2	0.0685	0.0008	0.0010
3 3 3	0.0755	-0.0003	-0.0001

TABLE II. Structure factors (absolute values) of the total charge density of Si [e/atom].

G	LDA	GW	Exp.
1 1 1	10.7210	10.7157	10.713
2 2 0	8.6536	8.6501	8.655
3 1 1	8.0205	8.0182	8.027
4 0 0	7.4414	7.4423	7.454
3 3 1	7.2256	7.2277	7.246
4 2 2	6.6984	6.6992	6.712
3 3 3	6.4086	6.4083	6.420

TABLE III. Structure factors (absolute values) of the pseudo valence charge density of Ge [e/atom] at LDA level and the correction from the GW approximation with and without adjusting the Hartree potential.

G	LDA valence	$\Delta\rho$ (V_H GW)	$\Delta\rho$ (V_H LDA)
1 1 1	1.3181	-0.0169	-0.0239
2 2 0	0.0035	-0.0086	-0.0107
3 1 1	0.2201	-0.0036	-0.0033
4 0 0	0.2052	0.0025	0.0037
3 3 1	0.0974	0.0037	0.0040
4 2 2	0.0865	0.0027	0.0033
3 3 3	0.0726	0.0017	0.0023

TABLE IV. Structure factors (absolute values) of the total charge density of Ge [e/atom].

G	LDA	GW	Exp.
1 1 1	27.5205	27.5036	27.453
2 2 0	23.6819	23.6734	23.677
3 1 1	22.1675	22.1639	22.138
4 0 0	20.3205	20.3230	20.273
3 3 1	19.4545	19.4582	19.509
4 2 2	18.0361	18.0388	18.066
3 3 3	17.2916	17.2939	17.315

TABLE V. Quasi-particle energies of Si [eV].

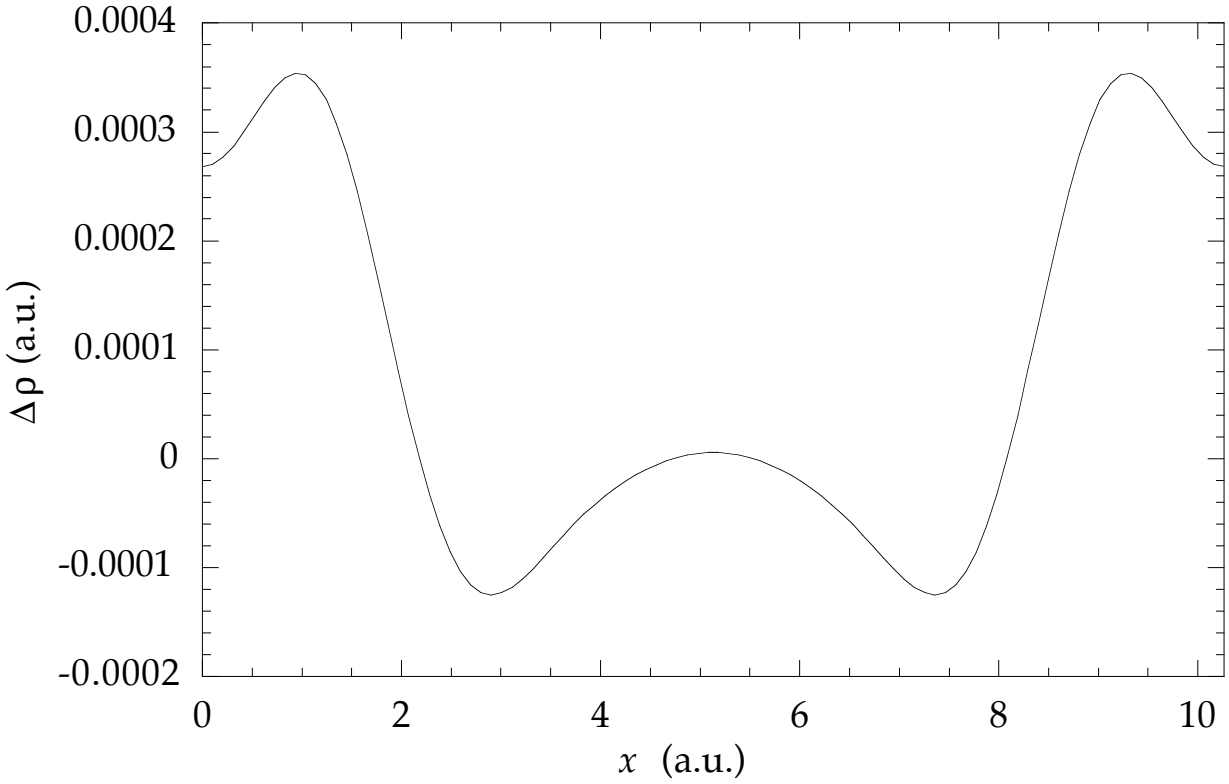
level	LDA	$GW + \mathrm{V}_H^{LDA}$	$GW + \mathrm{V}_H^{GW}$	Exp.
Γ_{1c}	-11.88	-11.91	-11.91	-12.50
$\Gamma_{25'v}$	0.00	0.00	0.00	0.00
Γ_{15c}	2.59	3.26	3.26	3.05
$\Gamma_{2'c}$	3.26	4.05	4.03	4.1
X_{1v}	-7.77	-7.88	-7.88	-8.18
X_{4v}	-2.81	-2.92	-2.92	-2.9
X_{1c}	0.62	1.24	1.25	1.25
X_{4c}	10.11	11.00	10.99	10.95
$L_{2'v}$	-9.56	-9.64	-9.64	-9.3
L_{1v}	-6.95	-7.09	-7.08	-6.7
$L_{3'v}$	-1.16	-1.22	-1.22	-1.2
L_{1c}	1.46	2.14	2.14	1.65
L_{3c}	3.34	4.07	4.08	4.15
$L_{2'c}$	7.73	8.34	8.36	
Gap	0.49	1.10	1.11	1.17

TABLE VI. Quasi-particle energies of Ge [eV].

level	LDA	$GW + \mathrm{V}_H^{LDA}$	$GW + \mathrm{V}_H^{GW}$	Exp.
Γ_{1c}	-12.63	-12.79	-12.79	-12.60
$\Gamma_{25'v}$	0.00	0.00	0.00	0.00
$\Gamma_{2'c}$	0.01	0.66	0.63	0.89
Γ_{15c}	2.61	3.11	3.14	3.21
X_{1v}	-8.83	-8.97	-8.98	-9.3
X_{4v}	-2.98	-3.11	-3.09	-3.15
X_{1c}	0.68	1.08	1.12	1.3
X_{3c}	9.56	10.32	10.32	
$L_{2'v}$	-10.61	-10.76	-10.76	-10.6
L_{1v}	-7.54	-7.69	-7.68	-7.7
$L_{3'v}$	-1.35	-1.40	-1.40	-1.4
L_{1c}	0.14	0.64	0.66	0.74
L_{3c}	3.77	4.29	4.32	4.3
$L_{2'c}$	7.24	7.65	7.73	7.8

FIG. 1. Difference between the GW and LDA charge densities[7] of Si (atomic units) along the edge of a conventional cell between two atom sites. Distance in Bohr radii. The GW correction slightly increases the concentration of electrons between the atoms.

FIG. 2. Difference between the GW and LDA charge densities[7] of Ge (atomic units) along the edge of a conventional cell between two atom sites. Distance in Bohr radii. The GW correction slightly increases the concentration of electrons between the atoms.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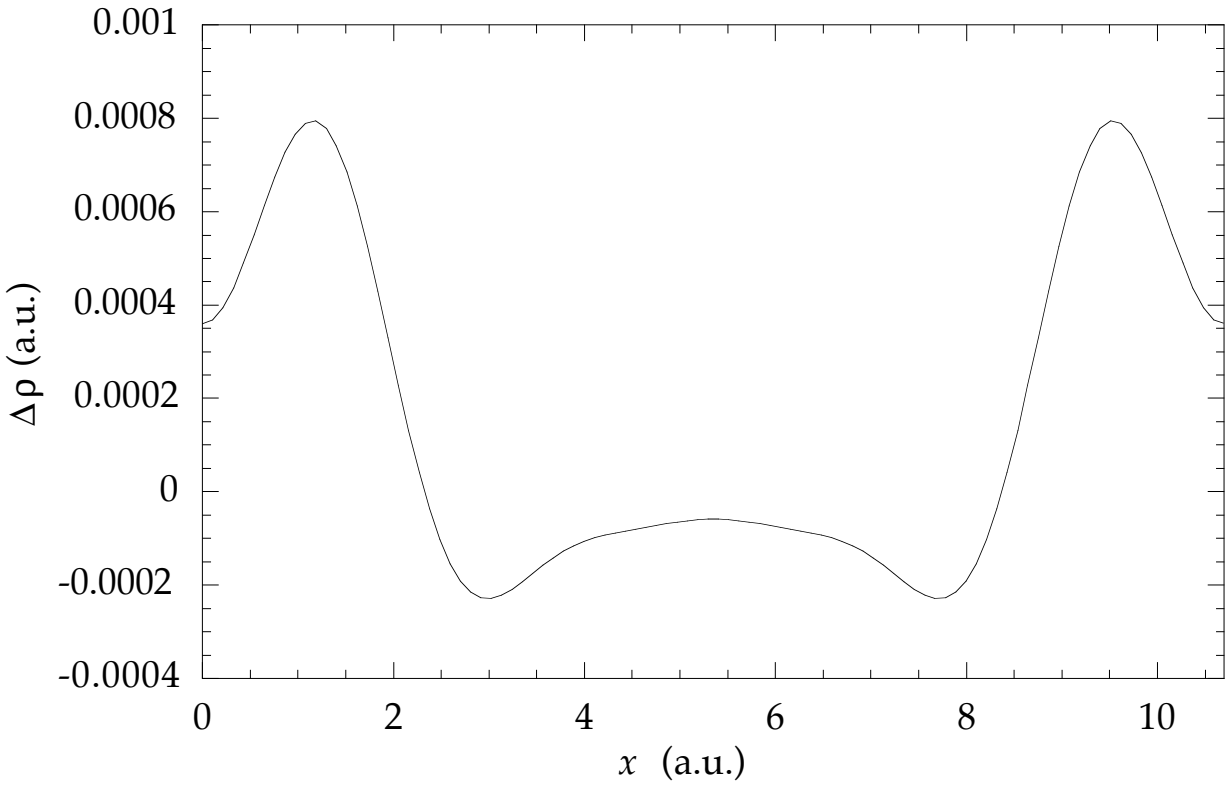
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