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**Finite Temperature Quasiparticle Self-Consistent GW Approximation**

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# Finite Temperature Quasiparticle Self-Consistent GW Approximation

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## Abstract

We present a new *ab initio* method for electronic structure calculations of materials at finite temperature (FT) based on the all-electron quasiparticle self-consistent GW (QPscGW) approximation and Keldysh time-loop Green's function approach. We apply the method to Si, Ge, GaAs, InSb, and diamond and show that the band gaps of these materials universally decrease with temperature in contrast with the local density approximation (LDA) of density functional theory (DFT) where the band gaps universally increase. At temperatures of a few eV the difference between quasiparticle energies obtained in FT-QPscGW and FT-LDA approaches significantly reduces. This result suggests that existing simulations of very high temperature materials based on the FT-LDA are more justified than it might appear from well-known LDA band gap errors at zero-temperature.

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## **Table of Contents**

Introduction.....	7
Theoretical Approach.....	9
Results.....	11
Conclusion.....	12
References.....	13
Figures.....	14

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# Finite temperature quasiparticle self-consistent GW approximation

## I. INTRODUCTION

Recent developments in a wide variety of fields, including dense plasmas [1], inertial confinement fusion [2], and astrophysics [3], require an improved understanding of the electrical and optical properties of various media at temperatures of a few to several tens of eV, when matter becomes partly dissociated, ionized, and degenerate. At such complex conditions, reached experimentally by shock compression in the Mbar range [1], laser heating of solid targets [4], or exploding wires [5], many-body effects are essential and standard semi-classical atomic physics models quickly becomes unreliable [6]. This region of phase space is often referred to as warm dense matter and has been the subject of considerable interest in recent years, driven by experimental programs in high energy density physics (HEDP). To improve our understanding of materials under these conditions, quantum molecular dynamics (QMD) simulations have been used recently [7], where for a statistically independent set of instantaneous atomic positions obtained from QMD the detailed electronic structure and electrical and optical conductivity were calculated within the finite temperature LDA (FT-LDA), which employs finite temperature Fermi distribution for calculation of the electron density and standard LDA potential. However, a well-known deficiency of the LDA is the systematic underestimation of the band gap in insulators and semiconductors. At high temperatures the conduction band is partly thermally occupied and any errors in the FT-LDA band gap directly affects the electron population of the conduction band, and, correspondingly, the calculated electrical and optical conductivity, and other properties [8].

The *GW* approximation of Hedin [9] is a natural way to describe the many-body electron interactions at the level beyond DFT. It is known [10–12] that the *GW* method generates very accurate band structures of materials at zero temperature with typical error  $\lesssim 0.2$  eV compared to experiment, while typical error of LDA-DFT is  $\sim 1$  eV. In this paper we develop a new *ab initio* method for electronic structure calculations of materials at finite electronic temperature based on Keldysh time-loop Green's function approach and the all-electron quasiparticle self-consistent *GW* (QPsc*GW*) approximation developed in our previous works [11–13]. Here we do not consider effects of electron-phonon interactions and thermal expansion assuming fixed positions of atoms. In conjunction with QMD that describes the motion of atoms this method can be applied to the above

problems of HEDP. Also, with simple modifications, this method can be applied to simulation of materials with electrons excited from valence bands to conduction bands by ultrashort pulsed laser and help to understand results of recent pump-probe experiments (see, e.g. [14]) at times prior to ion motion. Additionally, this method allows one to calculate the electronic contribution to the band gap temperature dependence of materials, thus serving as a benchmark for evaluating the accuracy of FT-LDA.

We applied our method to five materials with a wide range of band gaps (InSb, Ge, Si, GaAs, and diamond) and explore fundamental questions regarding how the band gaps and quasiparticle (QP) energy levels vary with electronic temperature in the  $GW$  approach and how this compares with the FT-LDA (in both approaches we interpret the Kohn-Sham eigenvalues spectrum as an electron spectrum). To the best of our knowledge these are the first such FT- $GW$  calculations of the band gaps for semiconductors and insulators. We show that the  $GW$  band gaps universally decrease with temperature, in contrast with the FT-LDA where the band gaps universally increase. At temperatures of a few eV the difference between the FT- $GW$  and FT-LDA quasiparticle energy levels is significantly reduced compared to that at zero temperature. This is an important result showing that existing high temperature calculations based on the FT-LDA are more justified than it might appear from the known LDA band gap errors at zero-temperature. Still, the  $GW$  calculations are required to achieve 0.1eV accuracy for calculated QP levels.

Because the  $GW$  method has severe demands in both its implementation and computation, *further* approximations are usually employed which significantly affect results. Almost ubiquitous is the one-shot  $GW$  where the self-energy is computed using LDA wave functions. Also the self-energy is usually computed from valence electrons only, omitting core contributions; or a pseudopotential (PP) constructed from the LDA replaces the core [10]. Only recently, when reliable all-electron implementations have begun to appear, has it been shown that the one-shot  $GW$  with PP leads to systematic errors [15]. Our all-electron quasiparticle self-consistent  $GW$  approach [11, 12] does not exploit the LDA, shape, or pseudopotential approximations in the construction of the potential; basically, no important approximation is made other than the  $GW$  approximation itself. We showed [11, 12] that the QP energies and other electronic properties of more than 30 materials calculated at zero temperature are in excellent agreement with experiments (typical error of band gap is  $\lesssim 0.2$  eV).



## II. THEORETICAL APPROACH

We now turn to the theory of the FT-*GW* method. Self-consistency in our FT-QPsc*GW* method is achieved by iterations. We start with some initial hermitian and energy independent self-energy  $\Sigma_{xc}$  (converged results do not depend on the initial  $\Sigma_{xc}$ ) and solve the Kohn-Sham equation for QP wave functions  $\psi_n^{\mathbf{k}}$  and energies  $\varepsilon_n^{\mathbf{k}}$ :

$$\left(-\frac{\nabla^2}{2m} + V_n + V_H - \varepsilon_n^{\mathbf{k}}\right)\psi_n^{\mathbf{k}}(\mathbf{r}) + \int d\mathbf{r}' \Sigma_{xc}^{\mathbf{k}}(\mathbf{r}, \mathbf{r}')\psi_n^{\mathbf{k}}(\mathbf{r}') = 0, \quad (1)$$

where  $V_n$  and  $V_H$  are nuclei and Hartree potentials,  $\mathbf{k}$  is the wave vector, and  $n$  is the band index. The four Keldysh components (retarded, advanced, lesser, and greater) of the Green's function for the system in equilibrium at finite temperature  $T$  are given by [16, 17]

$$G^{r/a}(\mathbf{r}, \mathbf{r}', \omega) = \sum_{n, \mathbf{k}} \psi_n^{\mathbf{k}}(\mathbf{r})\psi_n^{\mathbf{k}*}(\mathbf{r}') \frac{1}{\omega - \varepsilon_n^{\mathbf{k}} \pm i0} \quad (2)$$

$$G^{</>}(\omega) = \frac{\pm 1}{1 + \exp[\pm(\omega - \varepsilon_F)/T]} [G^a(\omega) - G^r(\omega)],$$

where  $\varepsilon_F$  is the Fermi energy. We use the system of units where  $\hbar = k = 1$ .

The polarization operator is calculated within the random-phase approximation,  $\Pi(\mathbf{r}, \tau; \mathbf{r}', \tau') = -iG(\mathbf{r}, \tau; \mathbf{r}', \tau')G(\mathbf{r}', \tau'; \mathbf{r}, \tau)$ , where  $\tau$  and  $\tau'$  are times on Keldysh time-loop contour [16, 17]. Using the Langreth rules [18, 19]  $[A(\tau, \tau')B(\tau', \tau)]^{r/a} = A^{r/a}(\tau, \tau')B^{<(\tau', \tau) + A^{<(\tau, \tau')B^{a/r}(\tau', \tau)$  and  $[A(\tau, \tau')B(\tau', \tau)]^{</>} = A^{</>}(\tau, \tau')B^{>(<(\tau', \tau)$  one can obtain the Keldysh components of  $\Pi$ :

$$\Pi_{IJ}^{r/a}(\mathbf{q}, \omega) = \sum_{\mathbf{k}, m, n} \left\langle M_I^{\mathbf{q}} \psi_n^{\mathbf{k}} | \psi_m^{\mathbf{k}+\mathbf{q}} \right\rangle \left\langle \psi_m^{\mathbf{k}+\mathbf{q}} | \psi_n^{\mathbf{k}} M_J^{\mathbf{q}} \right\rangle$$

$$\times \frac{[f(\varepsilon_n^{\mathbf{k}}) - f(\varepsilon_m^{\mathbf{k}+\mathbf{q}})]}{\omega - \varepsilon_m^{\mathbf{k}+\mathbf{q}} + \varepsilon_n^{\mathbf{k}} \pm i0} \quad (3)$$

$$\Pi_{IJ}^{</>}(\mathbf{q}, \omega) = \pm \frac{\Pi_{IJ}^a(\mathbf{q}, \omega) - \Pi_{IJ}^r(\mathbf{q}, \omega)}{1 - \exp(\pm\omega/T)}, \quad (4)$$

where  $f(\varepsilon) = 1/(1 + \exp[(\varepsilon - \varepsilon_F)/T])$  is the Fermi distribution function,  $M_I^{\mathbf{q}}$  are functions of mixed basis [13], and summation is taken over all bands and all momenta in the first Brillouin zone. Applying the Langreth rules [18, 19]  $(AB)^{r/a} = A^{r/a}B^{r/a}$  and  $(AB)^{</>} = A^r B^{</>} + A^{</>} B^a$  for time convolved Keldysh objects to a chain of products of the polarization operator  $\Pi$  and bare Coulomb potential  $V$ , one can obtain the Keldysh components of the screened Coulomb potential  $W_{IJ}(\mathbf{k}, \omega)$ :

$$W^{r/a} = \frac{1}{1 - V\Pi^{r/a}} V \quad (5)$$

$$W^{</>} = \frac{1}{1 - V\Pi^r} V \Pi^{</>} V \frac{1}{1 - \Pi^a V}.$$

In the  $GW$  approximation the exchange-correlation self-energy is given by  $\Sigma_{xc}(\mathbf{r}, \tau; \mathbf{r}', \tau') = iG(\mathbf{r}, \tau; \mathbf{r}', \tau')W(\mathbf{r}, \tau; \mathbf{r}', \tau')$ . The energy-independent matrix elements of exchange self-energy  $\Sigma_x = iG^<V$  are

$$\begin{aligned} \Sigma_{x,nn'}(\mathbf{q}) = & - \sum_{\mathbf{k}, I, J, m} \langle \psi_n^{\mathbf{q}} | \psi_m^{\mathbf{q}-\mathbf{k}} M_I^{\mathbf{q}} \rangle \\ & \times \langle M_J^{\mathbf{q}} \psi_m^{\mathbf{q}-\mathbf{k}} | \psi_{n'}^{\mathbf{q}} \rangle V_{IJ}(\mathbf{q}) f(\varepsilon_m^{\mathbf{q}-\mathbf{k}}). \end{aligned} \quad (6)$$

The retarded correlation self-energy  $\Sigma_c = iGW_c$  is

$$\begin{aligned} \Sigma_{c,nn'}^r(\mathbf{q}, \omega) = & \sum_{\mathbf{k}, I, J, m} \langle \psi_n^{\mathbf{q}} | \psi_m^{\mathbf{q}-\mathbf{k}} M_I^{\mathbf{q}} \rangle \langle M_J^{\mathbf{q}} \psi_m^{\mathbf{q}-\mathbf{k}} | \psi_{n'}^{\mathbf{q}} \rangle \\ & \times [-W_{c,IJ}^r(\mathbf{k}, \omega - \varepsilon_m^{\mathbf{q}-\mathbf{k}}) f(\varepsilon_m^{\mathbf{q}-\mathbf{k}}) \\ & + i \int \frac{d\omega'}{2\pi} \frac{W_{c,IJ}^>(\mathbf{k}, \omega')}{\omega - \omega' - \varepsilon_m^{\mathbf{q}-\mathbf{k}} + i0}], \end{aligned} \quad (7)$$

where  $W_c = W - V$ . Here we used the Langreth rule [18, 19]  $[A(\tau, \tau')B(\tau, \tau')]^r = A^r(\tau, \tau')B^<(\tau, \tau') + A^>(\tau, \tau')B^r(\tau, \tau')$  and Eq. (2) for retarded and lesser Green's functions. Applying Eq. (4) to (5) one finds

$$W^>(\omega) = \frac{1}{1 - \exp(-\omega/T)} [W^r(\omega) - W^a(\omega)]. \quad (8)$$

The function  $W^{r/a}(\omega')$  does not have a singularity in the upper/lower half-plane of the complex variable  $\omega'$ . Closing the integration contour of the integral  $\int d\omega' W^{r/a}(\omega')/[1 - \exp(-\omega'/T)]/[\omega - \omega' - \varepsilon_m^{\mathbf{q}-\mathbf{k}} + i0]$  in the upper/lower half-plane for  $W^{r/a}(\omega')$  we obtain

$$\begin{aligned} \Sigma_{c,nn'}^r(\mathbf{q}, \omega) = & \sum_{\mathbf{k}, I, J, m} \langle \psi_n^{\mathbf{q}} | \psi_m^{\mathbf{q}-\mathbf{k}} M_I^{\mathbf{q}} \rangle \langle M_J^{\mathbf{q}} \psi_m^{\mathbf{q}-\mathbf{k}} | \psi_{n'}^{\mathbf{q}} \rangle \\ & \times \{ W_{c,IJ}^r(\mathbf{k}, \omega - \varepsilon_m^{\mathbf{q}-\mathbf{k}}) \left[ \frac{1}{1 - e^{(\varepsilon_m^{\mathbf{q}-\mathbf{k}} - \omega)/T}} \right. \\ & \left. - f(\varepsilon_m^{\mathbf{q}-\mathbf{k}}) \right] - W_{c,IJ}^r(\mathbf{k}, 0) \frac{T}{\omega - \varepsilon_m^{\mathbf{q}-\mathbf{k}}} - 2T \\ & \left. \times \sum_{l=1}^{\infty} \frac{W_{c,IJ}^r(\mathbf{k}, i2\pi l) (\omega - \varepsilon_m^{\mathbf{q}-\mathbf{k}})}{(2\pi l T)^2 + (\omega - \varepsilon_m^{\mathbf{q}-\mathbf{k}})^2} \right\}. \end{aligned} \quad (9)$$

Here we used the time reversal symmetry  $W_{c,IJ}^a(\mathbf{k}, \omega) = W_{c,IJ}^r(\mathbf{k}, -\omega)$  and the equality  $\frac{1}{1 - \exp(-\omega'/T)} = \sum_{l=-\infty}^{\infty} \frac{T}{\omega' - i2\pi l}$ . At  $T \rightarrow 0$  the  $l$ -summation in Eq. (9) becomes an integration and  $\Sigma_c^r$  (9) reduces, at  $\omega > \varepsilon_F$ , to the correct time-ordered zero-temperature correlation self-energy [13].

At the final step of the iteration cycle we make the static and hermitian operator [11, 12]  $\Sigma_{xc}^{\mathbf{q}}(r, r') = \sum_{nn'} |\psi_n^{\mathbf{q}}\rangle (\Sigma_{x,nn'}(\mathbf{q}) + \Sigma_{c,nn'}(\mathbf{q})) \langle \psi_{n'}^{\mathbf{q}}|$ , where

$$\Sigma_{c,nn'}(\mathbf{q}) = \text{Re}[\Sigma_{c,nn'}^r(\mathbf{q}, \varepsilon_n^{\mathbf{q}}) + \Sigma_{c,nn'}^r(\mathbf{q}, \varepsilon_{n'}^{\mathbf{q}})]/2. \quad (10)$$

Here  $Re$  means that we take only hermitian part. We show elsewhere that the choice of Eq. (10) is not *ad hoc* but is reasonable approximation to the optimum construction of the QP Hamiltonian [12]. The obtained  $\Sigma_{xc}^q(r, r')$  defines the next-iteration Kohn-Sham equation (1); and the process is repeated until self-consistency. The spin-orbital coupling was added to the converged QP hamiltonian in first order of the perturbation theory.

### III. RESULTS

Fig 1. shows the band structure calculated by FT-QPscGW and FT-LDA methods at zero (left panels) and finite (right panels)  $T$  for InSb, Ge, Si, GaAs, and diamond. At zero  $T$  the QPscGW excitation spectrum for all five materials is in excellent agreement with experimental data with typical error  $\lesssim 0.2$  eV, while the LDA error is of the order of  $\sim 1$  eV (similar results for band gaps of large collection of materials at zero  $T$  are presented in Ref. [12]). The right panels of Fig. 1 show that the difference between all QP energy levels calculated by FT-LDA and FT-QPscGW becomes much smaller at  $T$  of several eV compared to zero  $T$ . This is one of the main results of this paper. This result can be explained by the fact that at high  $T$  the electrons occupy high-energy delocalized states, the electron density becomes more homogeneous compared to that at zero  $T$ , and the LDA potential, derived from exchange-correlation functional of homogeneous electron gas, becomes more accurate.

Fig. 2 shows the temperature dependence of the fundamental band gaps  $E_g^{GW}$  and  $E_g^{LDA}$  for five materials calculated by FT-QPscGW and FT-LDA approaches (top panel) and the difference  $E_g^{GW} - E_g^{LDA}$  (bottom panel). The steady increase of the FT-LDA band gaps with  $T$  for Si, Ge, and diamond can be explained by the fact that at high  $T$  electrons populate conduction states and induce changes in the Hartree potential that counteract the additional excitation of the valence electrons by increasing the QP energy of conduction states. For GaAs and InSb analogous change in the Hartree potential causes the increase of the gap up to  $T \sim 1$  eV as electrons are moved from the top of valence band near As and Sb to the bottom of conduction band near Ga and In. At even higher  $T$  some electrons are excited from semicore  $d$  levels of Ga and In (at  $\sim 18$  eV below the Fermi energy) causing compensation to initial charge polarization and downturn of the FT-LDA gaps of GaAs and InSb with increasing  $T$ .

The  $GW$  band gaps show qualitatively different behavior, with fast initial reduction with  $T$  and more slow behavior at larger  $T$ . The initial fast reduction of the gaps can be explained as follows. At zero  $T$  the absolute values of (negative) diagonal matrix elements of  $\Sigma_x$  (6) for the occupied

states are larger than for unoccupied states. At high  $T$  the occupied and unoccupied states are not distinguished any more, so the difference between diagonal matrix elements of  $\Sigma_x$  for “occupied” and “unoccupied” states reduces, resulting in reduction of the  $GW$  band gap. Also, the presence of Fermi factors in polarization operator (3) increases screening that leads to additional reduction of the band gap with  $T$ . The decrease of the gap by these factors dominates until the electrostatic term becomes important, as seen from the upturn of the diamond gap at  $T \sim 110$  kK and sign reversal of the second derivative of the  $GW$  gap for GaAs and InSb at  $T \sim 33$  kK. The bottom panel of Fig. 2 shows that  $E_g^{GW} - E_g^{LDA}$  initially reduces rapidly with  $T$  and tends to saturate at higher  $T$ . At  $T = 20$  kK the difference  $E_g^{GW} - E_g^{LDA}$  is at least two times smaller than that at zero  $T$  and lays in the interval  $\pm 0.5$  eV at  $T$  from 30 kK to 50 kK for all studied materials.

The  $GW$  band gap of all materials is open at the temperatures studied, except InSb, whose gap closes at  $T = 12.5$  kK. Up to 20% of valence  $sp$  electrons of GaAs are moved to the conduction bands for the temperature range shown on Fig. 2, but the gap is still open. This result contradicts empirical PP calculations [20] that predict closure of the gap at  $\sim 10\%$  level of excited  $sp$  electrons, but is in agreement with optical pump-probe experiment [14] predicting that there is no band gap closure due to electron excitations, and recent PP  $GW$  calculations [21] that use quasi-Fermi levels in conduction and valence bands to describe the electron occupation.

#### IV. CONCLUSION

In summary, we developed a new *ab initio* method for electronic structure calculations at finite temperature based on the all-electron quasiparticle self-consistent  $GW$  approximation and Keldysh time-loop Green’s function approach. We apply the method to Si, Ge, GaAs, InSb, and diamond and show that at temperatures of a few eV the difference between QP energies obtained in FT-QPsc $GW$  and FT-LDA approaches is significantly reduced. This result might serve as a justification of FT-LDA applicability to simulations of warm dense matter and as a useful foundation for correcting FT-LDA band gaps. These results are of considerable importance for HEDP because it remains numerically very challenging to use approaches beyond FT-LDA for description of many atoms in large unit cells employed in HEDP simulations.

## References

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- [1] G. W. Collins *et al.*, *Science* **281**, 1178 (1998).
- [2] J. D. Lindl *et al.*, *Phys. Today* **45**(9), 32 (1992).
- [3] C. A. Iglesias *et al.*, *Astrophys. J. Lett.* **569**, L111 (2002).
- [4] B. J. Siwick *et al.*, *Science* **302**, 1382 (2003).
- [5] V. Recoules *et al.*, *Phys. Rev E* **66**, 056412 (2002).
- [6] T. Blensky, *Astrophys. J., Suppl. Ser.* **127**, 239 (2000).
- [7] S. Mazevet *et al.*, *Phys. Rev. E* **71**, 016409 (2005) and references therein.
- [8] M. P. Desjarlais *et al.*, *Phys. Rev E* **66**, 025401(R) (2002).
- [9] L. Hedin, *Phys. Rev.* **139**, A796 (1965).
- [10] M. S. Hybertsen and S. Louie, *Phys. Rev B* **34**, 5390 (1986).
- [11] S. V. Faleev, M. van Schilfgaarde, and T. Kotani, *Phys. Rev. Lett.* **93**, 126406 (2004).
- [12] M. van Schilfgaarde, T. Kotani, and S. V. Faleev, submitted to *Nature Physics* (2005).
- [13] T. Kotani and M. van Schilfgaarde, *Sol. State Commun.* **121**, 461 (2002).
- [14] H. Huang *et al.*, *Phys. Rev. Lett.* **80**, 185 (1998).
- [15] M. van Schilfgaarde, T. Kotani, and S.V. Faleev, cond-mat/0508295 (2005), and references therein.
- [16] L. V. Keldysh, *J. Exp. Theor. Phys.* **47**, 1515 (1964).
- [17] J. Rammer, *Rev. Mod. Phys.* **58**, 323 (1986).
- [18] D. C. Langreth, in *Linear and Nonlinear Electron Transport in Solids*, edited by J. T. Devreese and E. Van Doren (Plenum, New York, 1976).
- [19] H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, Berlin, 1996).
- [20] D.H. Kim *et al.*, *Solid State Commun.* **89**, 119 (1994).
- [21] C.D. Spataru *et al.*, *Phys. Rev. B* **69**, 205204 (2004).

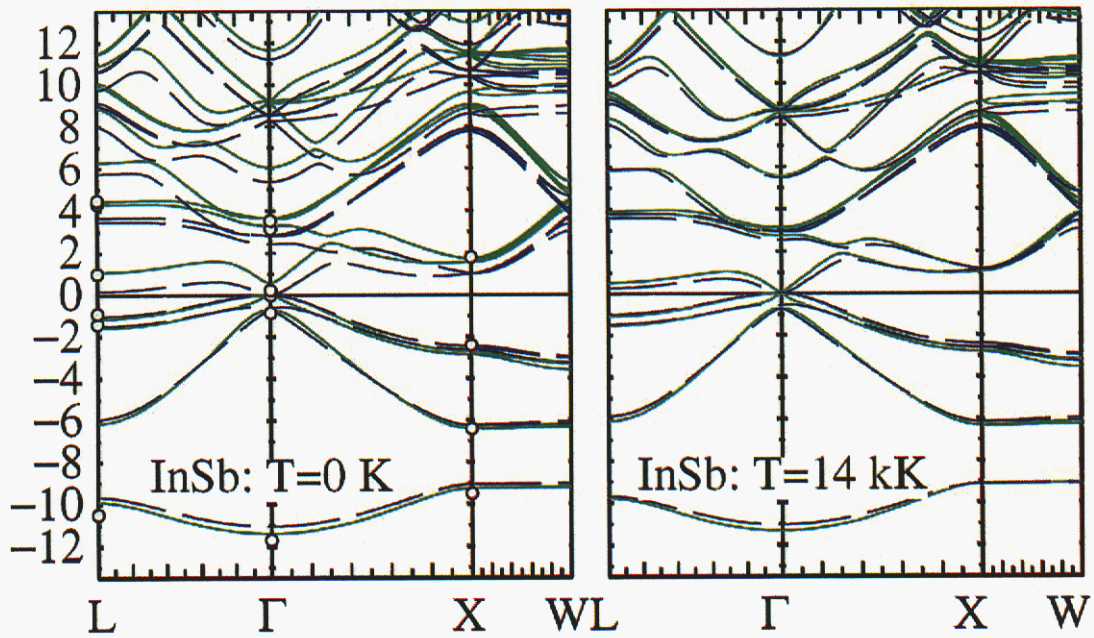


Figure 1a. Band structure of InSb calculated by QPscGW (full line) and LDA (dashed line) at temperatures shown. Experimental points are shown as open circles.

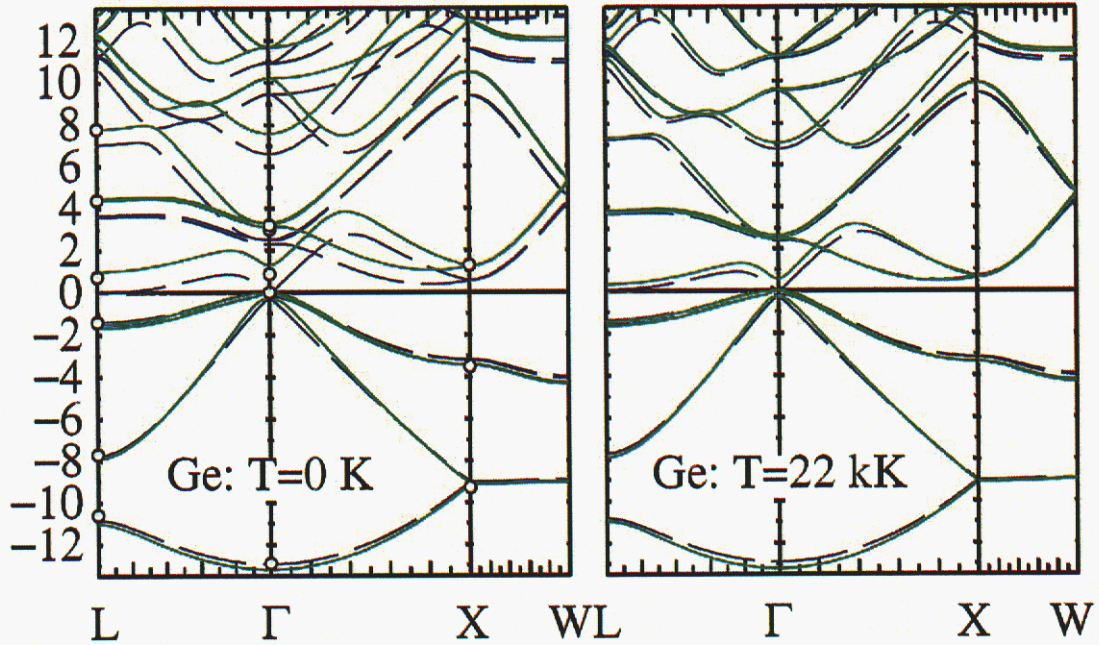


Figure 1b. Band structure of Ge calculated by QPscGW (full line) and LDA (dashed line) at temperatures shown. Experimental points are shown as open circles.

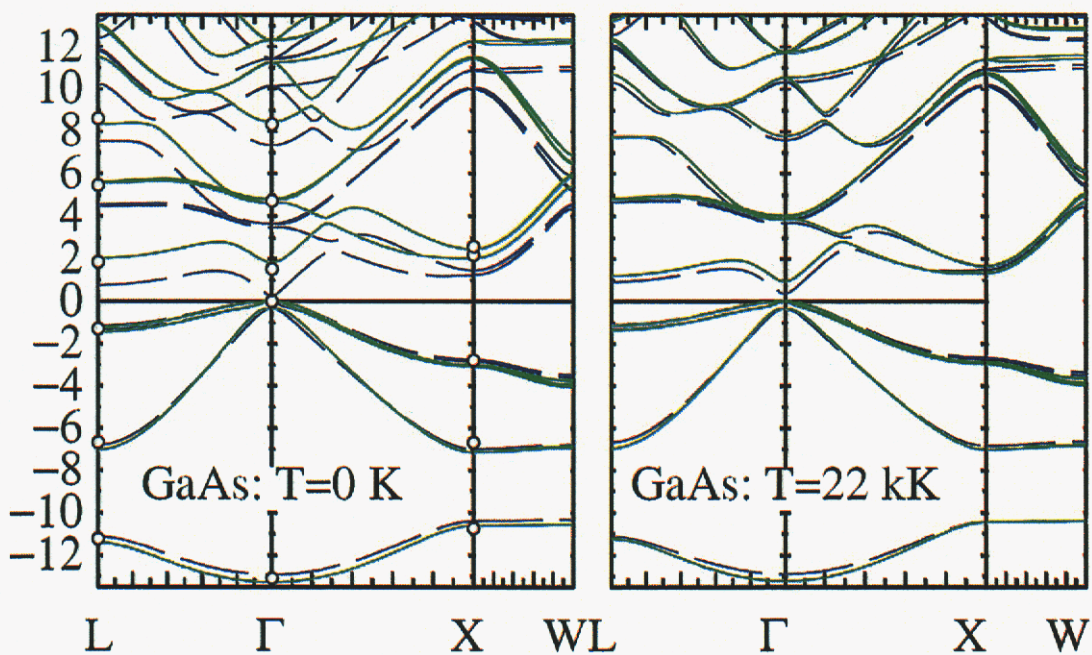


Figure 1c. Band structure of GaAs calculated by QPscGW (full line) and LDA (dashed line) at temperatures shown. Experimental points are shown as open circles.

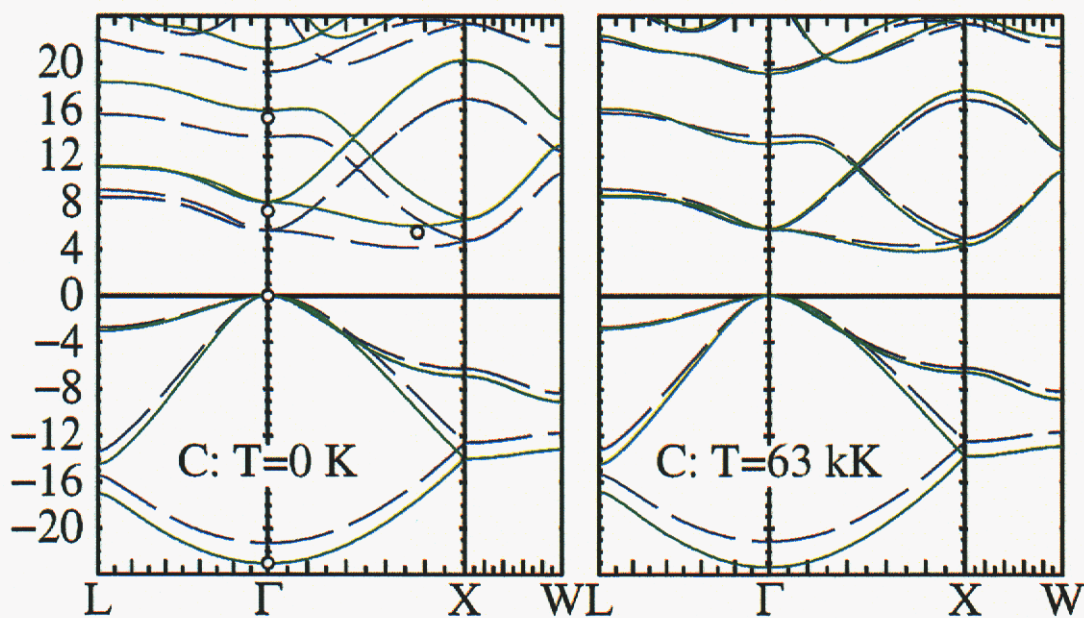


Figure 1d. Band structure of diamond calculated by QPscGW (full line) and LDA (dashed line) at temperatures shown. Experimental points are shown as open circles,

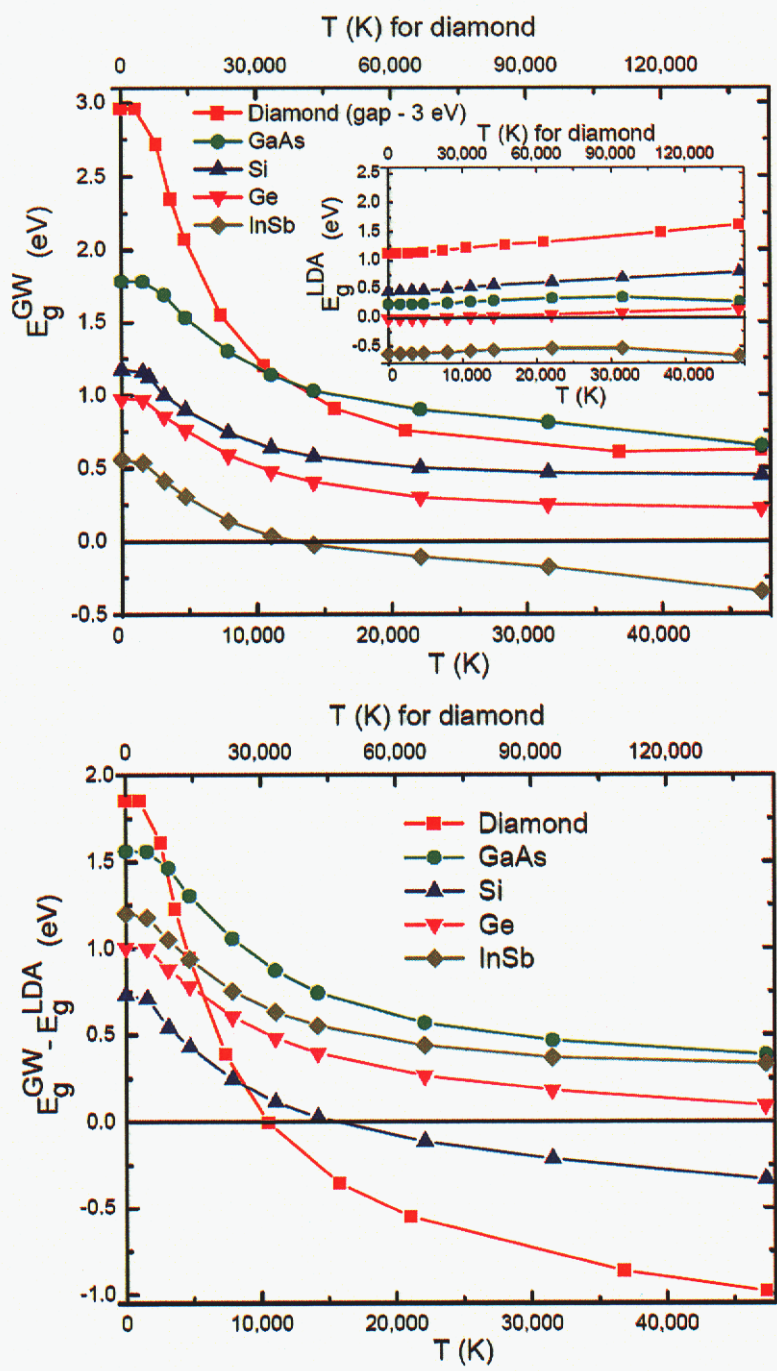


Figure 2. Upper panel: fundamental band gaps of five materials calculated in QPscGW approach as function of electronic temperature. For better scaling 3 eV has been subtracted from gap of diamond (note different temperature scale for diamond). Insert: LDA band gaps. Bottom panel: difference between QPscGW and LDA fundamental band gaps as function of temperature.



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