Understanding band gaps of solids in generalized Kohn–Sham theory

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The fundamental energy gap of a periodic solid distinguishes insulators from metals and characterizes low-energy single-electron excitations. However, the gap in the band structure of the exact multiplicative Kohn–Sham (KS) potential substantially underestimates the fundamental gap, a major limitation of KS density-functional theory. Here, we give a simple proof of a theorem: In generalized KS theory (GKS), the band gap of an extended system equals the fundamental gap for the approximate functional if the GKS potential operator is continuous and the density change is delocalized when an electron or hole is added. Our theorem explains how GKS band gaps from metageneralized gradient approximations (meta-GGAs) and hybrid functionals can be more realistic than those from GGAs or even from the exact KS potential. The theorem also follows from earlier work. The band edges in the GKS one-electron spectrum are also related to measurable energies. A linear chain of hydrogen molecules, solid aluminum arsenide, and solid argon provide numerical illustrations.

Significance

Semiconductors and insulators have a fundamental energy gap and absorb light at a continuum of photon energies above this gap. They also have a band structure of one-electron energies, and a band gap separating unoccupied from occupied one-electron states. When should these gaps be equal? It is known that they are not equal in the exact Kohn–Sham density-functional theory but are equal in commonly used density-functional approximations, such as the generalized gradient approximation (GGA). We show here that they are also equal (and improved) in higher level approximations, such as the meta-GGA or the hybrid of GGA with exact exchange, when the effective one-electron potential is not constrained to be a multiplication operator.


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the difference between the lowest-unoccupied (LU) and highest-occupied (HO) one-electron energies. We show here that under common computational conditions for solids, $g$ equals $G$ for a given approximate functional. How close $g$ is to the experimental gap depends on how accurate the functional is for the ground-state energy difference $G$ (strongly and comparably underestimated by LSDA and GGAs, but better estimated by meta-GGAs and especially hybrids).

In principle, should the band gap $g$ equal the fundamental energy gap $G$? In the early 1980s, band-structure calculations were accurate enough to show that LSDA band gaps for semiconductors were often about half the measured fundamental energy gaps. Was this a failure of the LSDA effective potential to mimic the exact KS potential, or an inability of the exact KS potential (for the neutral solid) to predict the fundamental gaps, or both?

Regarding the fundamental gap $G$ as an excitation energy, we do not expect it to equal the band gap $g$ of the exact KS potential. But, thinking of it as a ground-state energy difference, we might hope that it is. Williams and von Barth (9) gave a clear argument to support this hope, based on three assumptions: (i) Janak’s theorem (10, 11): The one-electron energies of KS theory are derivatives of the total energy with respect to occupation number, between integer occupations, in both finite and extended systems. This is unquestionably true. (ii) When an electron is added to or removed from a solid, the density change is infinitesimal and periodic. This assumption, only possible for an extended system, is often true, although there may be exceptions in which added electrons or holes get stuck in localized states; see refs. 12 and 13 for possible examples. (iii) When an electron is added or removed, the KS potential changes only infinitesimally. This assumption seemed to follow so naturally from (ii) that it was only implicit in the argument, yet assumption (iii) is incorrect for the exact KS potential.

Other work (14–17) of the early 1980s showed that the exact KS potential jumps up by an additive-constant discontinuity when an electron is added to a neutral solid, making

$$G_{\text{exact}} = g_{\text{exact}} + xc_{\text{discontinuity}}.$$  

The discontinuity spoils the interpretation of $g$, shifting the one-electron energies without changing the density. The KS potential is a mathematical fiction, acting on noninteracting electrons to yield the true ground-state density of the neutral solid and making the one-electron energy for the highest partly occupied one-electron state equal to the true chemical potential $\mu = dE/dM$, which is itself discontinuous at zero temperature for an insulator when $M$ crosses $N$. The xc discontinuity is absent in the LSDA and GGA approximations to the multiplicative xc potential, for which (17)

$$G_{\text{approx}} = g_{\text{approx}}.$$  

In Eq. 4, $G$ of Eq. 1 and $g$ of Eq. 2 are evaluated with the same approximate functional. Whereas GGA improves ground-state energies and electron densities over LSDA, both approximations yield nearly the same band gaps $g$ and hence fundamental gaps $G$, excepting some special GGAs (18). It has long been known (17) that Eq. 4 is true in LSDA and GGA, and it has been suspected (e.g., refs. 15 and 17) that LSDA and GGA band gaps are close to exact KS band gaps (but not to true fundamental gaps).

**Band-Gap Problem in Generalized KS Theory**

A simple, self-contained proof of our theorem will be given here. Refs. 19–22 by themselves also imply this result, as discussed in a later section.

Based mostly upon empiricism, realistic fundamental gaps for semiconductors (e.g., refs. 23 and 24) have been estimated from band gaps of hybrid functionals in generalized KS (GKS) theory, which is also an excellent starting point for simple quasi-particle corrections (25). A global hybrid replaces a fraction [e.g., 25% (7, 26, 27)] of GGA exchange with that of Hartree–Fock, and replaces the same fraction of the GGA exchange potential with that of Hartree–Fock (an integral operator, not a multiplication operator). Screened hybrids (e.g., ref. 8) additionally screen the interelectronic Coulomb potential in the exchange term, and typically improve results for semiconductors (23).

We argue that Eq. 4 is also valid within typical approximations in GKS theory, as typically implemented, extending the argument of Williams and von Barth (9) from KS to GKS theory. Thus, the improvement in the band gap that comes from using a hybrid functional reflects a corresponding improvement in the value for $G$ of Eq. 1. Our detailed argument, presented in Appendix B: Theoretical Methods, generalizes assumption (i) of the Williams–von Barth argument (9) from KS to GKS theory, and notes that the GKS potentials, like the LSDA and GGA and unlike the exact one, have no discontinuity under change of particle number, consistent with refs. 19–22.

Although there is a formally exact GKS theory (28), here we view GKS as a small step out of KS theory, in which one can use nonempirical approximations to $E_x$ that are constructed to satisfy the known exact constraints of KS theory. In rigorous KS density-functional theory, the occupied KS one-electron states are demonstrably implicit functionals of the electron density that can be used to construct a density-functional approximation, such as an explicit functional of the KS one-electron density matrix. For example, use the noninteracting kinetic energy density to construct a meta-GGA (e.g., ref. 5), or use the full KS density matrix to construct the Hartree–Fock exchange energy for a global hybrid as in ref. 7. Because the one-electron states are only implicit functionals of the density, the KS potential can be constructed only by the optimized effective potential (OEP) method (29). It is computationally easier to find the variationally optimized potential that minimizes the energy with respect to the noninteracting density matrix. The resulting GKS potential is not a multiplication operator but is in practice continuous (does not change when one delocalized electron is added to or subtracted from a solid) and self-adjoint for differentiable functionals of the noninteracting density matrix. It is an integral (Fock) operator (11) for hybrids but a differential operator (30, 31) for meta-GGAs, the same operator for occupied and unoccupied one-electron states.

The step outside KS to GKS barely affects the occupied one-electron states, the electron density, and the total energy, but not so the one-electron energies. This was first shown by comparing exchange-only OEP (KS) and Hartree–Fock (GKS) results for atoms (29, 32), and more recently by comparing the corresponding KS and GKS implementations of meta-GGAs (exchange and correlation together) for atoms (33) and solids (31). They produce closely similar results for total energies, but the KS meta-GGA band gap is close to that of LSDA and GGA, whereas the GKS meta-GGA band gap is significantly larger and more realistic.

Within xc approximations using the noninteracting density matrix, relaxing the KS demand for a multiplicative effective potential is a “practical” approximation with an unexpected benefit: It yields the interpretation of Eq. 4 for the GKS band gap of a solid, explaining how meta-GGAs and especially hybrids can improve the estimation of the fundamental energy gap of a solid:
For a typical approximate functional, the GKS band gap $g$ is the ground-state energy difference $G$. Improvements in $G$ correlate at least roughly with other improvements in ground-state energy differences for integer electron numbers, relevant to atomization energies and lattice constants.

**Numerical Demonstration**

Because computational effort typically scales like the cube of the number of atoms, finite 3- and even 2D clusters are much harder to converge to the mesoscopic length scale, so we consider as a first model a finite 1D linear chain of realistic $\text{H}_2$ molecules. The separation between the nuclei of neighboring molecules is taken to be 1.25Å, the separation between nuclei within a molecule (0.74 Å), to produce a gap of order 3 or 4 eV. To demonstrate our conclusions, the model does not need to be realistic, and its exact gap does not need to be known. With an even number of molecules, the model does not need to be realistic, and its fundamental gaps of real extended solids from a given functional electron affinity as the chain length grows. In contrast to the resonances (forming polarons) can be captured by a related supercell approach (39). A self-consistent calculation for the neutral system yields a band gap $g$ and an energy $E(N)$. Removal of one electron from the HOrbital or one-electron state (the $k$-point at the top of the valence band), while keeping the other occupations and orbitals unchanged, yields the non-self-consistent $E_{\text{non-SCF}}(N - 1)$, whereas allowing orbital relaxation yields the self-consistent $E_{\text{SCF}}(N - 1)$. Contributions to the Hartree energy and Hartree potential from the zero reciprocal lattice vector are not taken into account in the charged systems, or (as usual) in the neutral ones. This known approach for charged systems (40) is better justified for bulk periodic solids than for other cases (41). Thus, without any code modification, a finite energy $E(N - 1)$ is obtained. An ionization potential $I(N)$ is just the difference $E(N - 1) - E(N)$, where neither energy is divided by the number of primitive unit cells. An energy $E(N + 1)$ is obtained analogously by adding one electron to the $k$ point representing the bottom of the conduction band. From Eq. 1 the fundamental energy gaps $G_{\text{non-SCF}}$ and $G_{\text{SCF}}$, for the cases without and with orbital relaxation, respectively, are calculated. Convergence with mesh size is rapid.

![Fig. 1. PBE GGA fundamental gap $G$ and band gap $g$ for a linear chain of $N_{\text{mol}}$ $\text{H}_2$ molecules. Note that $G$ converges to the limit $N_{\text{mol}} \to \infty$ much more slowly than $g$ does.](image)

**Table 1.** Ionization energy $I$, electron affinity $A$, and fundamental gap $G = I - A$ of an infinite linear chain of $\text{H}_2$ molecules, evaluated by extrapolation from finite chains, and the band edges $-\varepsilon^{\text{HO}}$, $-\varepsilon^{\text{LU}}$ and band gap $g = -\varepsilon^{\text{LU}} - -\varepsilon^{\text{HO}}$ in the LSDA (2), PBE GGA (4), SCAN meta-GGA (5), and HSE06 range-separated hybrid (8) functionals

<table>
<thead>
<tr>
<th>Method</th>
<th>$I$ (eV)</th>
<th>$A$ (eV)</th>
<th>$G$ (eV)</th>
<th>$g$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LSDA</td>
<td>1.65</td>
<td>3.14</td>
<td>3.13</td>
<td>0.16</td>
</tr>
<tr>
<td>PBE</td>
<td>1.67</td>
<td>3.24</td>
<td>3.23</td>
<td>0.09</td>
</tr>
<tr>
<td>SCAN</td>
<td>1.68</td>
<td>3.33</td>
<td>3.31</td>
<td>0.01</td>
</tr>
<tr>
<td>HSE06</td>
<td>1.82</td>
<td>3.92</td>
<td>3.91</td>
<td>-0.29</td>
</tr>
</tbody>
</table>

The extrapolated band energies agree closely with those from a periodic-boundary-condition calculation (shown). $(I+A)/2$, the energy difference from the gap center to the vacuum level (15), depends only weakly on the approximation.

![Fig. 2. Difference between the fundamental gap $G = I - A$ and the GKS band gap $g = -\varepsilon^{LU} - -\varepsilon^{HO}$ for a linear chain of $N_{\text{mol}}$ hydrogen molecules.](image)
as in ref. 36, they can be transformed into approximate quasiparticle band structures.

Conclusions

The fundamental energy gap is the most basic property of a periodic solid. It cannot be found from a single KS band-structure calculation, even with the unattainable exact density functional. Surprisingly, high-level approximations, implemented in an efficient generalized KS scheme, yield band gaps equal to the fundamental gap for a given approximate functional. Future all-purpose nonempirical approximate functionals could predict usefully correct gaps for most solids. The band edges (43) in the GKS one-electron spectrum, relevant to interface formation and redox catalysis, can also be interpreted as measurable energy differences, as shown by Eq. 6 and illustrated in Table 1. They can be found in principle by extrapolating the GKS one-electron energies of a slab or cluster.

Typical approximate functionals, as typically implemented, obey Eq. 4, as previously known (17) only for LSDA and GGA. For 3D solids (31), there is little or no improvement in $G_{\text{approx}}$ from LSDA to GGAs, but substantially more from GGAs to fully nonlocal functionals, where the nonlocality of the density dependence and the usefulness of the band gap $G_{\text{approx}}$ increase further from meta-GGAs to hybrids. This suggests that, in solids, the xc effects can be more long-ranged (e.g., ref. 23) than in atoms and small molecules.

The PBE0 and Heyd–Scuseria–Ernzerhof 2006 (HSE06) hybrids contain 25% of exact exchange, globally or at intermediate range, chosen to yield accurate atomization energies for molecules and related moderate-gap systems at integer electron number. The nonlinear variation of approximate total energy with electron number between adjacent integers is a problem in finite systems, but vanishes in typical solids (1, 20). PBE0 and especially HSE06 yield realistic GKS gaps for typical semiconductors. But, they can over- or underestimate gaps of other solids. For example, molecular crystals seem to need $1/\epsilon$ of long-range exact exchange (44), where $\epsilon$ is the dielectric constant (45).

Appendix A: Computational Methods

The self-consistent all-electron results for the chain of hydrogen molecules reported here were found using the Gaussian code (46) with a small cc-pvdZ basis set, to speed up the hybrid calculations for the longer chains. Many results were checked with the ADF (47) (TZP basis) and FHI-aims (48) (NAO-VCC-22 basis) codes. The effect of increasing the basis from cc-pvdZ to TZP is to increase the $N_{\text{nl}} \rightarrow \infty$ limits of $I$ and $A$ in PBE by 0.14 and 0.10 eV, respectively.

Table 2. KS (PBE) and OEP/KS and GKS (PBE0) band gap $g$ and fundamental energy gaps $G$ of solid AlAs, calculated according to Eq. 1 with orbitals of the neutral $N$-electron system $G_{\text{non-SCF}}$, or with orbitals of separate self-consistent calculations of $N$, $(N - 1)$, and $(N + 1)$-electron systems $G_{\text{SCF}}$, in electron volts, as described in the text.

$$\begin{array}{cccccc}
\text{Grid size} & g & g_{\text{non-SCF}} & g_{\text{SCF}} & g_{\text{OEP}} & g \\
2 \times 2 \times 2 & 1.62 & 1.54 & 1.53 & 1.52 & 1.51 \\
2 \times 4 \times 4 & 1.32 & 1.31 & 1.30 & 1.29 & 1.28 \\
4 \times 6 \times 6 & 1.34 & 1.34 & 1.34 & 1.33 & 1.33 \\
8 \times 8 \times 8 & 1.34 & 1.34 & 1.34 & 1.33 & 1.33 \\
10 \times 10 \times 10 & 1.34 & 1.34 & 1.34 & 1.33 & 1.33 \\
12 \times 12 \times 12 & 1.34 & 1.34 & 1.34 & 1.33 & 1.33 \\
\end{array}$$

The experimental band gap (52) of AlAs is 2.23 eV.

Table 3. KS(PBE) and OEP/KS and GKS(PBE0) band gap $g$ and fundamental energy gaps $G$ of solid Ar, calculated according to Eq. 1 with orbitals of the neutral $N$-electron system $G_{\text{non-SCF}}$, or with orbitals of separate self-consistent calculations of $N$, $(N - 1)$, and $(N + 1)$-electron systems $G_{\text{SCF}}$, in electron volts, as discussed in the text.

$$\begin{array}{cccccc}
\text{Grid size} & g & g_{\text{non-SCF}} & g_{\text{SCF}} & g_{\text{OEP}} & g \\
1 \times 1 \times 1 & 7.62 & 7.62 & 7.62 & 7.62 & 7.62 \\
2 \times 2 \times 2 & 8.64 & 8.64 & 8.64 & 8.64 & 8.64 \\
3 \times 3 \times 3 & 8.68 & 8.68 & 8.68 & 8.68 & 8.68 \\
4 \times 4 \times 4 & 8.69 & 8.69 & 8.69 & 8.69 & 8.69 \\
5 \times 5 \times 5 & 8.69 & 8.69 & 8.69 & 8.69 & 8.69 \\
6 \times 6 \times 6 & 8.69 & 8.69 & 8.69 & 8.69 & 8.69 \\
7 \times 7 \times 7 & 8.69 & 8.69 & 8.69 & 8.69 & 8.69 \\
8 \times 8 \times 8 & 8.69 & 8.69 & 8.69 & 8.69 & 8.69 \\
\end{array}$$

The experimental band gap (53) of Ar is 14.20 eV. For a recent comparison of GKS band gaps for many solids from GGA hybrid functionals, including PBE0 and HSE, see ref. 54.
respectively, and to stabilize the negative-ion resonances for some of the larger finite chains. All codes show $G - g = \cdots - 0.02 \text{ eV}$, which we attribute to the slow convergence of $G$ with increasing system size (Fig. 1). All extrapolations display the increase of $J$ and decrease of $A$ from LSDA to HSE06.

The ALAs and Ar calculations were carried out with the plane-wave program MCEXX (49) using norm-conserving PBE pseudopotentials generated by the code of ref. 50, which is based on the Troullier–Martins scheme (51). The cutoffs used for the construction of the pseudopotentials are the same as those used in ref. 37. In principle, the pseudopotential for PBE should be different from that for PBE, but the difference is irrelevant to our demonstration. For ALAs a lattice parameter of 5.66 Å and a plane-wave cutoff of 15 a.u. were used. The corresponding values for Ar were 5.26 Å and 30 a.u.

**Appendix B: Theoretical Methods**

Here we derive the generalized Janak theorem and prove that the band gap and band edges of generalized KS theory are the appropriate ground-state energy differences, for a given approximate functional. In any constrained minimization, the Lagrange multiplier is the derivative of the minimized quantity with respect to the value of the constraint. Consider minimizing the orbital functional $E_i(\{f_i\}, \{\psi_i\})$, where $n_i = \int f_i^2 \psi_i^2$ and the occupation numbers are restricted to the range $0 \leq n_i \leq 1$ with $\sum_i n_i = N$, subject to constraints $\int f_i \Delta \psi_i \psi_i^2 = 0$ guaranteeing normalization of the occupied or partly occupied orbitals. The Euler–Lagrange equation for this problem is $\delta E_i(\{f_i\}, \{\psi_i\}) = \sum_i n_i \delta f_i \Delta \psi_i \psi_i^2 = 0$, where the $e_i$ are Lagrange multipliers. The interpretation is $e_i = \delta E/\delta f_i$. [5]

This is a generalized Janak theorem. The same statement and derivation (11) apply to the ungeneralized KS theory. The minimizing one-electron wave-functions are solutions of an one-electron Schrödinger equation with an optimal variational potential operator.

Consider a GKS calculation for an extended solid with an approximate xc functional, in which the ground state delocalizes the density of the added electron over the whole solid. The variation of the approximated $E$ is linear in $f$, because the relaxation effect on the optimal variational potential associated with the removal or addition of one electron is negligible. Then, by Eq. 5,

$$E(N) - E(N-1) = \epsilon_H^0(N-\delta)$$

where $\delta = 0$, and

$$I(N) = A(N) = \epsilon_H^0(N+\delta) - \epsilon_H^0(N-\delta).$$

For a meta-GGA or hybrid functional, the optimum variational potential operator has been found explicitly (e.g., equation 7 of ref. 30; equation 1.7 of ref. 11) and is continuous. Thus, within LSDA, GGA, meta-GGA, or hybrid approximations, when implemented in GKS, the band gap equals the ground-state total energy difference.

In contrast, within an ungeneralized KS scheme, this statement remains true in LSDA and GGA, but not in meta-GGA or hybrid approximations. For meta-GGA and hybrid approximations, treated in OEP, for (15) exact KS theory,

$$I(N) = A(N) = \epsilon_H^0(N+\delta) - \epsilon_H^0(N-\delta)$$

where the first set of curly brackets is the OEP or KS band gap and the second set is the contribution from the discontinuity (15, 16) of the OEP or KS potential.

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$$\Delta E(\{\psi_i\}, \{f_i\}) = \sum_i n_i \delta f_i \Delta \psi_i \psi_i^2 = 0$$

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