Comment on "Band-Gap Problem in Semiconductors Revisited: Effects of Core States and Many-Body Self-Consistency"

In a recent Letter [1], Ku and Eguiluz concluded that deep-core states and many-body self-consistency have an important effect on the theoretical band gap in semiconductors, based on their calculations for bulk Si and Ge. Their conclusions question the validity of pseudopotentials in *GW* calculations, claiming that this approach is successful due to a previously unknown error cancellation. We address two points raised by the Letter: first, which approximation for the self-energy operator is best used for electronic-structure calculations, and, second, the use of pseudopotentials.

It is clear from the iterative expansion of Hedin's equations [2] that the *GW* approximation does not yield the complete self-energy. Neglected are vertex corrections and, in most cases, a self-consistent solution of Dyson's equation. Indeed, the self-energy within this so-called G_0W_0 approximation violates a number of sum rules including conservation of the particle number [3]. However, it has been demonstrated many times [4] that G_0W_0 gives excellent agreement with experiment for quasiparticle energies. In contrast, a self-consistent solution of Dyson's equation conserves the particle number, and has been found to improve ground state energies [5], but agreement with experiment for band structures worsens. It is generally understood that the omission of vertices and the lack of self-consistency tend to have opposing effects on the quasiparticle energy.

In order to clarify the confusion between the many approaches available, we have performed a range of highly converged calculations for isolated Be, Mg, and Ne atoms as prototype many-electron systems, including non-, partially, and fully self-consistent *GW* (with a *full* solution of Dyson's equation), using either a local-density approximation (LDA) Troullier-Martins pseudopotential or all electrons. These choices permit a direct test of one claim of Ku and Eguiluz: that core-valence exchange is inaccurate in G_0W_0 calculations. Computed ionization potentials (IPs) for the Be atom are presented in Table I. The IP is analogous to a gap in our calculations since a Be atom has no electron affinity, experimentally and within the *GW* approximation. It can be seen that the use of pseudopotentials does not significantly affect the IP obtained within any of the *GW* approximations. It is also clear that a self-consistency destroys the agreement with experiment, with a vertex function then required to repair the IP. We observe similar trends for Ne and Mg atoms. These results do not suggest any further cancellation of errors between the use of pseudopotentials and the lack of a self-consistent solution, and therefore do not support the conclusions of Ku and Eguiluz.

Furthermore, the initial Green's function used to form the self-energy operator includes a sum over the complete infinite set of unoccupied states from a separate noninteracting calculation. In practice this sum is truncated. Testing the validity of the truncation is important; states with a surprisingly high energy are often required to provide an accurate numerical representation. As an example, all results in Table I required states up to 8–10 Ha above E_F to be included in G_0. By comparison, in Ref. [1] only states up to around 1.1 Ha above E_F were used. Applying the same cutoff to our atom calculations, all results are altered by more than 0.5 eV, changing the conclusions. These observations for the convergence are similar to those in a recent study for bulk semiconductors [6], demonstrating that this slow convergence is a common feature of a wide range of systems.

TABLE I. Ionization energy (in eV) of an isolated Be atom from the *GW* approximation. Experimental = 9.33 eV.

Method	All-electron	Pseudopotential
DFT-LDA	5.43	5.43
G_0W_0	9.25 ± 0.01	9.24 ± 0.01
GW_0	8.75 ± 0.01	8.75 ± 0.01
GW	8.47 ± 0.01	8.64 ± 0.01

In summary, the G_0W_0 approximation for the self-energy operator gives excellent quasiparticle energies. We have demonstrated that the pseudopotential method remains a valid numerical technique in many-body calculations, if the calculation is numerically converged.

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