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Recent Developments in Electronic Structure Methods: The Quasiparticle Self-Consistent GW Approximation[1]

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The ability to solve the fundamental equation of motion of condensed matter — the Schrodinger equation—from first principles, has evolved a great deal in the last 30 years. The standard workhorse, the Local Density Approximation (LDA) is now widely used in most branches of science and engineering. However, it has many limitations, and numerous attempts to extend and improve on the the LDA have been attempted. There have been notable successes, but most of these methods are semi-empirical, and tend to be specialized — suitable for resolving one or another failing of the LDA. Here we prsent a new type of approach based on Hedin's GW approximation. This approach, which we call the quasiparticle self-consistent *GW* (QS*GW*) approximation, is based on a kind of self-consistent perturbation theory, where the self-consistency is constructed to minimize the perturbation. QS*GW* describes optical properties in a wide range of materials rather well, including cases where the local-density and LDA-based *GW* approximations fail qualitatively. Self-consistency dramatically improves agreement with experiment, and is sometimes essential. QS*GW* avoids some formal and practical problems encountered in conventional self-consistent *GW*, which will be discussed. QS*GW* handles both itinerant and correlated electrons on an equal footing, in a true *ab initio* manner without any ambiguity about how a localized state is defined, or how double-counting terms should be subtracted. Weakly correlated materials such as Na and *sp* semiconductors are described with uniformly high accuracy. Discrepancies with experiment are small and systematic, and can be explained in terms of the approximations made. Its consistently high accuracy make QS*GW* a versatile method that can reliably predict critical energy band properties of GaAs, $CuInSe_2$, TiO_2 and NiO in a unified framework.

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