Efficient GW Method Based on an Enhanced Static Approximation

Wei Kang and Mark S. Hybertsen

Center for Functional Nanomaterials, Brookhaven National Laboratory
Upton, NY, USA

The unfavorable scaling of calculations based on the GW approach with system size impedes many applications. Recent efforts to eliminate the explicit use of empty states in the calculations represent one approach to this problem. Another approach is to improve approximations based on physical interpretation. We have analyzed the static Coulomb-hole and screened exchange (COHSEX) approximation proposed by Hedin and find that most of its errors derive from the short wavelength contributions to the Coulomb-hole (COH) term. The origin of these errors can be traced back to the "adiabatic" accumulation of the screened Coulomb interaction that is assumed. In our new method, a "non-adiabatic" correction to the static COHSEX model is described by a wavenumber-dependent multiplicative factor in the COH term. We show that this factor can be approximated by a single scaling function, determined from the homogeneous electron gas model. The local field effect in real materials is captured by a simple ansatz based on symmetry considerations. Our new method inherits the efficiency of the static COHSEX. Tests for a series of crystals and molecules are surprisingly accurate suggesting that this approach may be very promising.