Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

The sc-COHSEX+GW and the static off-diagonal GW approaches to quasiparticle wavefunctions and energies JACK DESLIPPE, MANISH JAIN, GEORGY SAMSONIDZE, MARVIN COHEN, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Within the conventional GW approach, density functional theory (DFT) is typically used as a mean-field starting point; the self-energy operator is evaluated to 1st order in the DFT Green's function G_0 and screened Coulomb interaction W_0. The quasiparticle energies are calculated from diagonal elements of Σ in the DFT orbital basis. This approach works extraordinarily well for many materials but has limitations when the DFT states are far from the quasiparticle wavefunctions. In such cases, off-diagonal elements of Σ in the mean-field basis are large and the full Σ matrix is needed. The slow convergence of the off-diagonal elements make approaches requiring the explicit construction of this matrix prohibitively expensive. We present two alternative approaches based on the static (COHSEX) approximation that efficiently include the mean-field off-diagonal matrix element effects: a sc-COHSEX+GW approach where a renormalized basis is obtained from a self-consistent evaluation of quasiparticle wavefunctions in the static approximation and a less intensive treatment of just the off-diagonal elements within the COHSEX approximation. We show examples of the approaches for molecules and crystalline systems. Support by NSF DMR10-1006184, DOE DE-AC02-05CH11231.

Jack Deslippe
University of California at Berkeley and Lawrence Berkeley National Lab

Date submitted: 20 Dec 2010 Electronic form version 1.4