Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Constructing unoccupied states for G_0W_0 quasiparticle calculations from plane-waves GEORGY SAMSONIDZE, MANISH JAIN, JACK DESLIPPE, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Standard methods of first-principles calculations of the quasiparticle energies within the G_0W_0 scheme require summing over large numbers of unoccupied states. The generation of these states within the ab initio pseudopotential plane-wave density functional theory (DFT) quickly becomes a bottleneck of the calculation with increasing system size, especially in low-dimensional systems. In this work, we propose a method for approximating the high-energy continuum and resonant states in low-dimensional systems. The continuum and resonant states above a chosen energy are replaced with symmetrized plane-waves and localized DFT states computed with short-range localized basis functions (such as in the SIESTA code), respectively. The Gram-Schmidt process is used to orthogonalize these constructed high-energy unoccupied states. The method opens a route towards precise G_0W_0 quasiparticle calculations in large low-dimensional systems using a small number of unoccupied DFT states. This work was supported by NSF Grant No. DMR10-1006184, the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NSF through TeraGrid at NICS and DOE at LBNL's NERSC.

Georgy Samsonidze
Dept of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory,
Berkeley, CA 94720

Date submitted: 22 Dec 2010

Electronic form version 1.4