Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Efficient first principles quasiparticle states using optimal Brillouin zone sampling[1] DAVID PRENDERGAST, STEVEN G. LOUIE, Molecular Foundry, LBNL and Physics Dept, UC Berkeley — We present a methodology for accurate evaluation of quasiparticle states within the GW approximation [1], exploiting optimal Brillouin zone sampling [2]. This approach permits fast, efficient sampling of the Brillouin zone using a compact k-dependent Hamiltonian. Applications to systems with complicated dispersion or large numbers of atoms are permitted with favorable computational scaling and straightforward exploitation of existing parallelized numerical libraries. As input, this method requires only standard density functional theory calculations of eigenstates and eigenenergies on a very coarse k-point grid. For systems with large numbers of atoms, a single k-point is often sufficient. K-point convergence of the dielectric matrix and self-energy is readily achieved leading to accurate GW quasiparticle states. [1] M. S. Hybertsen and S. G. Louie, Phys. Rev. B **34**, 5390 (1986). [2] E. L. Shirley, Phys. Rev. B **54**, 16464 (1996).

[1]This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 and by National Science Foundation Grant No. DMR07-05941. Computational resources were provided by NERSC.

David Prendergast
Molecular Foundry, LBNL

Date submitted: 27 Nov 2007 Electronic form version 1.4