Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

The effect of semicore electrons on the polarizability and band gaps in *ab initio* planewave-pseudopotential (PW-PP) GW calculations[1]

DEREK VIGIL-FOWLER, University of California - Berkeley, Lawrence Berkeley National Laboratory, BRAD MALONE, Harvard University, STEVEN LOUIE, University of California - Berkeley, Lawrence Berkeley National Laboratory — Understanding the effect of semicore electrons on *ab initiio* PW-PP GW calculations is currently of great interest due to the increasing importance of complex materials with active semicore electrons, e.g.,the transition metal dichalcogenides. While past research has found a significant effect due to the inclusion of semicore electrons, it did not fully explore the nature of the various deviations of traditional valence-only PW-PP GW calculations from calculations that include the semicore electrons. We study this issue in the simple system of the Si atom, where the effect is more easily isolated, and then extend our results to bulk Si, and other bulk systems. We present results showing the effect of semicore electrons on various contributions to the GW self energy, and discuss the nature of differences with the traditional PW-PP approach. We present methods to efficiently include the effect of semicore electrons in a hierarchy of computational cost and accuracy.

[1]This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NERSC and NICS. D.V-F. acknowledges funding from the DOD's NDSEG fellowship.

Derek Vigil-Fowler
University of California - Berkeley, Lawrence Berkeley National Laboratory

Date submitted: 13 Nov 2013 Electronic form version 1.4