Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Single-particle and two-particle excited states with strong spin-orbit coupling[1] BRADFORD A. BARKER, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Many materials of interest have strong spin-orbit coupling, which necessitates the use of spinor wavefunctions in the calculation of their electronic and optical properties. We have implemented such spinor functionality in the BerkeleyGW code package to calculate from first principles single-particle excitations at the GW level and two-particle excitations at the GW-plus-Bethe Salpeter-Equation (GW-BSE) level. We present example calculations of benchmark materials with computational scaling details on the NERSC and TACC machines.

[1]The work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

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Date submitted: 11 Nov 2016 Electronic form version 1.4