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GW Calculations of Materials on the Intel Xeon-Phi Architecture[1] JACK DESLIPPE, LBNL, FELIPE H. DA JORNADA, UC Berkeley and LNBL, DEREK VIGIL-FOWLER, NREL, ARIEL BILLER, Weizmann Institute of Science, JAMES R. CHELIKOWSKY, UT Austin, STEVEN G. LOUIE, UC Berkeley and LBNL — Intel Xeon-Phi processors are expected to power a large number of High-Performance Computing (HPC) systems around the United States and the world in the near future. We evaluate the ability of GW and pre-requisite Density Functional Theory (DFT) calculations for materials on utilizing the Xeon-Phi architecture. We describe the optimization process and performance improvements achieved. We find that the GW method, like other higher level Many-Body methods beyond standard local/semilocal approximations to Kohn-Sham DFT, is particularly well suited for many-core architectures due to the ability to exploit a large amount of parallelism over plane-waves, band-pairs and frequencies.

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