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Large Scale GW Calculations on the Cori System¹ JACK DESLIPPE, MAURO DEL BEN, Lawrence Berkeley National Lab, FELIPE DA JORNADA, University of California, Berkeley and Lawrence Berkeley National Lab, ANDREW CANNING, Lawrence Berkeley National Lab, STEVEN LOUIE, University of California, Berkeley and Lawrence Berkeley National Lab — The NERSC Cori system, powered by 9000+ Intel Xeon-Phi processors, represents one of the largest HPC systems for open-science in the United States and the world. We discuss the optimization of the GW methodology for this system, including both node level and system-scale optimizations. We highlight multiple large scale (thousands of atoms) case studies and discuss both absolute application performance and comparison to calculations on more traditional HPC architectures. We find that the GW method is particularly well suited for many-core architectures due to the ability to exploit a large amount of parallelism across many layers of the system.

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