

Abstract Submitted
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Efficient First-principles Wang-Landau Calculations G. BROWN, Florida State University, A. RUSANU, KH. ODBADRAKH, M. EISENBACH, D.M. NICHOLSON, Oak Ridge National Laboratory — The Wang-Landau (WL) method of finding the density of states $g(E)$ contributing to the partition function $Z(kT)$ is useful for determining thermodynamic properties from first-principles energy calculations for magnetic systems. Since DFT calculations require significant computer resources, it is important to make the convergence of the WL method to a self-consistent $g(E)$ as efficient as possible. We present approaches for making accurate initial estimates of $g(E)$ based on similar Hamiltonians or estimates of $g(E)$ for a different number of atoms. These approaches can include workstation-based calculations using classical Heisenberg Hamiltonians based on exchange parameters calculated from initial data from DFT WL calculations. In addition, we announce several insights we have gained into the convergence of the WL method. For instance, the minimum curvature of the calculated $g(E)$ is limited by the update parameter and the maximum energy step of the Markov chain. This material is based upon work supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences. This research used resources of the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy.

Gregory Brown
Florida State U

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