**LSMS and WL-LSMS: Scalable ab initio calculations for materials**M. Eisenbach, Y. W. Li, Kh. Odbadrakh, X. Liu, Y. Wang
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**Abstract**

The Locally Self-consistent Multiple Scattering (LSMS) code solves the first principles Density Functional theory Kohn-Sham equation for a wide range of materials with a special focus on metals, alloys and metallic nanostructure and other materials applications. Additionally, WL-LSMS provides the capability to perform Wang-Landau Monte-Carlo sampling of magnetic and chemical order. This allows the first principles statistical physics calculation of magnetic and ordering phase transitions. By utilizing multiple Monte-Carlo walkers, the LSMS scalability is extended by multiple orders of magnitude. LSMS has traditionally exhibited near perfect scalability on massively parallel high performance computer architectures. It can exploit GPUs to accelerate the computations to enable first principles calculations of O(100,000) atoms and statistical physics sampling of finite temperature properties. Using the Cray XK7 system Titan at the Oak Ridge Leadership Computing Facility the LSMS code has demonstrated a sustained performance of 14.5PFlop/s and a speedup of 8.6 compared to the CPU-only code.

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