Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

An hybrid computing approach to accelerating the multiple scattering theory based *ab initio* methods[1] YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G. MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — The multiple scattering theory method, also known as the Korringa-Kohn-Rostoker (KKR) method, is considered an elegant approach to the *ab initio* electronic structure calculation for solids. Its convenience in accessing the one-electron Green function has led to the development of locally-self consistent multiple scattering (LSMS) method, a linear scaling *ab initio* method that allows for the electronic structure calculation for complex structures requiring tens of thousands of atoms in unit cell. It is one of the few applications that demonstrated petascale computing capability. In this presentation, we discuss our recent efforts in developing a hybrid computing approach for accelerating the full potential electronic structure calculation. Specifically, in the framework of our existing LSMS code in FORTRAN 90/95, we explore the many core resources on GPGPU accelerators by implementing the compute intensive functions (for the calculation of multiple scattering matrices and the single site solutions) in CUDA, and move the computational tasks to the GPGPUs if they are found available. We explain in details our approach to the CUDA programming and the code structure, and show the speed-up of the new hybrid code by comparing its performances on CPU/GPGPU and on CPU only.

[1]The work was supported in part by the Center for Defect Physics, a DOE-BES Energy Frontier Research Center.

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Date submitted: 14 Nov 2013 Electronic form version 1.4