Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

**Hybrid density functional calculation accelerated using GPGPU**
YOSHIHIDE YOSHIMOTO, Tottori University — Although hybrid density functionals are known to improve several simulated physical properties, their computational costs are very high because we have to compute the exchange interaction explicitly. For example, in plane wave based simulation programs, which are widely used, we have to execute a lot of Fast Fourier Transformation(FFT)s and this part becomes the majority of the cost. In this presentation, its acceleration using GPGPU implemented in the program package xTAPP will be presented. xTAPP is a plane wave based first principles calculation program package developed by the author and his collaborators. GPGPUs have very high memory band width which is required for FFTs. However the data transfer band width between a GPGPU and a CPU is rather low and this is the bottleneck to utilize GPGPU naively. In the xTAPP, this bottleneck is resolved by blocking the computation of the exchange interactions. The exchange interaction is an aggregate of band times band computations consists of FFTs. By blocking this computations with respect to the bands, we can reduce the proportion of data transfers between a CPU and a GPGPU to the computation of FFTs.

Yoshihide Yoshimoto
Tottori University

Date submitted: 15 Nov 2013 Electronic form version 1.4