Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Parallel performance for large scale GW calculation using the OpenAtom software[1] SUBHASISH MANDAL, MINJUNG KIM, Yale University, ERIC MIKIDA, KAVITHA CHNDRASEKAR, ERIC BOHM, University of Illinois Urbana-Champaign, NIKHIL JAIN, Lawrence Livermore National Laboratory, LAXMIKANT V. KALE, University of Illinois Urbana-Champaign, GLENN J. MARTYNA, IBM Thomas J. Watson Research Center, SOHRAB ISMAIL-BEIGI, Yale University — One of the accurate *ab initio* electronic structure methods that goes beyond density functional theory (DFT) to describe excited states of materials is GW-BSE method. Due to extreme computational demands of this approach, most *ab initio* GW calculations have been confined to small units of cells of bulk-like materials. We will describe our collaborative efforts to develop new parallel software that permits large scale and efficiently parallel GW calculations. Our GW software is interfaced with the open source ab initio plane wave pseudopotential OpenAtom software (http://charm.cs.uiuc.edu/OpenAtom/) that takes the advantage of Charm++ parallel framework. We will present our real-space computational approach, parallel algorithms and parallel scaling performance for the GW calculation and compare to other available open source software.

[1]This collaboration is supported by an NSF SI2-SSI grant (ACI-1339804).

Subhasish Mandal
Yale University

Date submitted: 11 Nov 2016 Electronic form version 1.4