abstract titled "Towards highly scalable GW calculations." These two talks are closely related to each other. We ask organizers to schedule these two presentations in the same session. It would be appreciated if this one could be presented first.

for the MAR16 Meeting of
The American Physical Society

Large-scale GW software development[1] MINJUNG KIM, SUBHASISH MANDAL, Department of Applied Physics, Yale University, ERIC MIKIDA, PRATEEK JINDAL, ERIC BOHM, NIKHIL JAIN, LAXMIKANT KALE, Department of Computer Science, University of Illinois at Urbana-Champaign, GLENN MARTYNA, IBM T. J. Watson Research Center, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Electronic excitations are important in understanding and designing many functional materials. In terms of *ab initio* methods, the GW and Bethe-Saltpeter Equation (GW-BSE) beyond DFT methods have proved successful in describing excited states in many materials. However, the heavy computational loads and large memory requirements have hindered their routine applicability by the materials physics community. We summarize some of our collaborative efforts to develop a new software framework designed for GW calculations on massively parallel supercomputers. Our GW code is interfaced with the plane-wave pseudopotential *ab initio* molecular dynamics software "OpenAtom" which is based on the Charm++ parallel library [1]. The computation of the electronic polarizability is one of the most expensive parts of any GW calculation. We describe our strategy that uses a real-space representation to avoid the large number of fast Fourier transforms (FFTs) common to most GW methods. We also describe an eigendecomposition of the plasmon modes from the resulting dielectric matrix that enhances efficiency. [1] Bohm *et al.*, IBM J. RES. & DEV. vol. 52 no. 1/2, 2008

[1]This work is supported by NSF through grant ACI-1339804.

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Date submitted: 06 Nov 2015 Electronic form version 1.4