Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Reduced order polarizability method for large scale GW calculations[1] MINJUNG KIM, SUBHASISH MANDAL, Yale University, ERIC MIKIDA, KAVITHA CHANDRASEKAR, ERIC BOHM, NIKHIL JAIN, LAXMIKANT KALE, University of Illinois at Urbana-Champaign, GLENN MARTYNA, IBM T. J. Watson Research Center, SOHRAB ISMAIL-BEIGI, Yale University — The GW method is an important tool for accurate calculation, from first principles, of excited electronic systems. However, the GW method has not been routinely applied to large scale materials physics or chemistry problems due to its heavy computational load and large memory requirements. The most computationally intense part of GW calculation is the calculation of the polarizability matrix: for standard "sum-over-states" approaches, it scales as N^4 where N is the number of electrons in the system. As part of our team's effort towards developing massively parallel GW software that can be readily applied to large-scale systems, we have implemented a real-space algorithm which greatly reduces the number of fast Fourier-transform to build polarizability matrix (in a plane wave basis). Using this real-space representation of the polarizability matrix, we are then able to develop two types of cubic-scaling polarizability methods that use interpolation or Gaussian quadrature to simplify the treatment of energy dependencies. We will describe the methods and their accuracies and efficiencies when applied to crystalline materials.

[1]This work is supported by National Science Foundation through grant ACI-1339084.

Minjung Kim
Yale Univ

Date submitted: 11 Nov 2016 Electronic form version 1.4