Abstract Submitted
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Towards highly scalable GW calculations[1] SUBHASISH MANDAL, MINJUNG KIM, Department of Applied Physics, Yale University, ERIC MIKIDA, ERIC BOHM, PRATEEK JINDAL, NIKHIL JAIN, Department of Computer Science, University of Illinois at Urbana Champaign, LAXMIKANT V. KALE, Department of Computer Science, University of Illinois at UrbanaChampaign, GLENN J. MARTYNA, IBM T. J. Watson Research Center, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — The GW and Bethe-Saltpeter Equation (GW-BSE) approach is an accurate and useful method beyond DFT to describe excited states of materials. However over the past few decades, most *ab initio* GW calculations used have been confined to small units of cells of bulk-like materials due to the extreme computational demands of the approach. We will present our collaborative efforts to develop new software that permits large scale GW calculations more efficiently: our GW software is interfaced with the ab initio plane wave pseudopotential OpenAtom software (http://charm.cs.uiuc.edu/OpenAtom/) that uses the Charm++ parallel framework. Here, we focus on describing our work on computing the static (so called "COHSEX) GW self-energy. We describe the advantages of our real-space approach for quasi-particle calculations and provide information on scaling behavior of the resulting algorithms.

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