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Implementation of highly parallel and large scale GW calculations within the OpenAtom software

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The need to describe electronic excitations with better accuracy than provided by band structures produced by Density Functional Theory (DFT) has been a long-term enterprise for the computational condensed matter and materials theory communities. In some cases, appropriate theoretical frameworks have existed for some time but have been difficult to apply widely due to computational cost. For example, the GW approximation (L. Hedin, *Phys. Rev.* **139**, 1965) incorporates a great deal of important non-local and dynamical electronic interaction effects but has been too computationally expensive for routine use in large materials simulations.

OpenAtom is an open source massively parallel *ab initio* density functional software package based on plane waves and pseudopotentials (http://charm.cs.uiuc.edu/OpenAtom/) that takes advantage of the Charm++ parallel framework. At present, it is developed via a three-way collaboration, funded by an NSF SI2-SSI grant (ACI-1339804), between Yale (Ismail-Beigi), IBM T. J. Watson (Glenn Martyna) and the University of Illinois at Urbana Champaign (Laxmikant Kale). We will describe the project and our current approach towards implementing large scale GW calculations with OpenAtom. Potential applications of large scale parallel GW software for problems involving electronic excitations in semiconductor and/or metal oxide systems will be also be pointed out.