

Abstract Submitted
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Speed-up of GW Full-Frequency Calculations using the Static Dielectric Matrix Subspace Approximation¹ MAURO DEL BEN, Lawrence Berkeley National Laboratory, FELIPE H. DA JORNADA, University of California at Berkeley and Lawrence Berkeley National Laboratory, JACK DESLIPPE, NERSC, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory, ANDREW CANNING, Lawrence Berkeley National Laboratory — Over the last several decades the GW method has been established as a quantitatively accurate approach for predicting the quasiparticle and excited-state properties of materials. However, the successful application of the method to large systems with thousands to tens-of-thousands of atoms is a challenge due to the computational complexity associated with the evaluation of the dielectric matrix ϵ and its frequency dependence. We describe the implementation in traditional GW calculations based on the expression of the frequency dependent part of ϵ on the subspace generated by selected eigenvectors of the static dielectric matrix. We validate the method with several benchmark calculations on molecules, slabs and bulk systems. We show that the overall accuracy of the method is solely determined by the threshold on the eigenvalues of the static ϵ and that excellent time to solution and speed-ups of an order of magnitude can be achieved without significant loss of accuracy.

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