

Abstract Submitted
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Plane wave based selfconsistent solution of the GW Dyson equation¹ LIN-WANG WANG, HUAWEI CAO, Lawrence Berkeley Natl Lab — We have developed a selfconsistent procedure to calculate the full Dyson equation based on plane wave basis set. The whole formalism is based on the Greens function matrix of the plane wave G-vector. There is no truncation of the conduction band when the dielectric function is calculated. The Dyson equation is the variational minimum solution of the total energy in terms of the Greens function. The calculation uses the "space-time" method, with special algorithm for imaginary time integration and Fourier transformation. We have tested isolated molecules and periodic systems. The effects of selfconsistency compared to the G0W0 results will be presented. We will also discuss some special techniques used in the k-point summation for the periodic system. Massive parallelization is used to carry out such calculations.

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