# The Gap-filling Method: $G_0W_0$ for Molecules

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## Abstract

There is a need to provide an efficient description of the electronic structure for the complex systems of chemistry. Mean field methods, such as Density Functional Theory (DFT), are the workhorse of the field because they offer decent accuracy at a cheap computational cost. Conversely, wavefunction-based methods, like Coupled Cluster theories (e.g., CCSD(T)), provide high accuracy at a steep computational cost. A middle ground is found with the GW approximation. Our focus is on the $G_0W_0$ variant of this method.

We describe an implementation of $G_0W_0$ and investigate properties of the recently proposed linearized $G_0W_0$ density matrix. Overall, we see a marked improvement in the treatment of electron correlation at a reasonable cost.