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**Combination of Hedin's $GW$ and dynamical mean-field theory tested on $H_2$ molecule** JUHO LEE, KRISTJAN HAULE, Rutgers University — We compare various flavors of "$GW$+DMFT" approach with LDA+DMFT for the simplest strongly correlated system, the $H_2$ molecule. The following $GW$+DMFT methodologies are compared: (i) the fully self-consistent GW+DMFT, (ii) the quasi-particle self-consistent QS-GW+DMFT with dynamic double-counting, (iii) QS-GW+DMFT with static double-counting schemes. We found that fully self-consistent $GW$+DMFT with exact double-counting yields very precise spectra around equilibrium H-H distance, as well as reasonable total energy (comparable to LDA+DMFT). However, this scheme breaks down in the correlated regime due to causality violation. The QS-GW+DMFT approaches, which are not derivable from a functional, yield similar spectra as full GW+DMFT near equilibrium distance, and in static double-counting schemes, can also be extended into correlated regime. However, the total energy of these approaches is much worse than the total energy of LDA+DMFT. In summary, this toy model of correlated physics suggests that QS-GW+DMFT with constant double-counting should give accurate predictions of spectra, but not total energy, while LDA+DMFT gives very precise total energy, but somewhat less precise spectra.

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