Tackling localized $d$-states: a systematic investigation by $GW@LDA+U$ Hong Jiang, Ricardo I. Gomez-Abal, FHI, Berlin, Germany, Patrick Rinke, UC Santa Barbara, USA, Matthias Scheffler, FHI, Berlin, Germany — First-principles modeling of systems with localized $d$-states is currently a great challenge in condensed matter physics. Density-functional theory (DFT) in the standard local-density approximation (LDA) proves to be problematic. This can be partly overcome by including local Hubbard $U$ corrections (LDA+$U$), but itinerant states are still treated on the LDA level. Many-body perturbation theory in the $GW$ approach offers both a quasiparticle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for localized states), and is therefore promising for these systems. Here we present a systematic investigation of the $G_0W_0$ method based on LDA+$U$ ($G_0W_0@LDA+U$) for a series of prototype systems: 1) ZnS with semicore $d$-states, 2) ScN and TiO$_2$ with empty $d$-states and 3) late transition metal oxides (MnO, FeO, CoO and NiO) with partially occupied $d$-states. We show that for ZnS, ScN and TiO$_2$, the $G_0W_0$ band gap only weakly depends on $U$, but for the other transition metal oxides the dependence on $U$ is as strong as in LDA+$U$. These different trends can be understood in terms of changes in the hybridization and screening. Our work demonstrates that $G_0W_0@LDA+U$ with “physical” values of $U$ provides a balanced and accurate description of both localized and itinerant states.

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