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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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