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Self-consistent GW(QP)+Vertex calculations for the insulating oxides of transition (rare earth) metals ANDREY KUTEPOV, VLADIMIR ANTROPOV, Ames Lab, Ames, IA, SERGEY SAVRASOV, University of California, Davis, CA, GABRIEL KOTLIAR, Rutgers University, Piscataway, NJ — Searching for a methodology with predictive power we have developed recently a new approach incorporating many-body vertex corrections into GW-based numerical schemes. Here we apply it to study the electronic structure of the following materials: SrTiO3, TiO2, NiO, and CeO2. We compare four different variations of the scheme: GW, GW+Vertex, QP (quasi-particle), and QP+Vertex. All calculations have self-consistency, at either the full or the QP level. Whereas vertex corrected GW approximation only partially corrects the GW results the QPGW approximation supplemented with first order vertex corrections to both polarizability and self energy allows us to improve essentially the agreement between calculated and experimental spectra. The addition of vertex correction diagrams to the GW method is straightforward. We discuss the subtleties involved in the addition of vertex corrections to the QPGW method. Formally our approach can be considered as fully self-consistent GW(QP)+DMFT method with a perturbative impurity solver and the implications for GW(QP)+DMFT will be discussed.

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