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GW for transition metal oxide perovskites ZEYNEP ERGONENC, BONGJAE KIM, PEITAO LIU, GEORG KRESSE, CESARE FRANCHINI, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — The *ab initio* calculation of quasiparticle (QP) energies is a technically and computationally challenging problem. In condensed matter physics the most widely used approach to determine QP energies is the *GW* approximation. Although the *GW* method has been widely applied to many typical semiconductors and insulators, its applications to more complex compounds such as $4d$ and $5d$ (and to a lesser extent $3d$) perovskites, have been comparatively rare, and its proper use is not well established from a technical point of view. In this work, we have applied the *GW* method to a representative set of transition-metal perovskites including $3d$, $4d$ and $5d$ compounds with different electron occupancies, magnetic ordering and structural characteristics. We will discuss the proper procedure to obtain converged QP energies and accurate bandgaps, and highlight the difference between norm-conserving and ultrasoft potentials in GW calculations.

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