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Improved LDA+U model for band gap corrected ZnO defect calculations ADISAK BOONCHUN, WALTER LAMBRECHT, Case Western Reserve University — The local density approximation (LDA) is known to fail dramatically for point defects in ZnO. In the case of the oxygen vacancy, the one electron level of the 1+ charge state lies above the conduction band and leads to improper filling of the levels. Different points of view on how to implement a-posterior gap corrections still leave large uncertainty on the position of the defect levels. For the Zn-vacancy, LDA leads incorrectly to a delocalized wave function of the hole on all four neighbors. Our approach is to apply LDA+U corrections to various orbitals, O-sp and Zn-spd. The U-parameters which lead to orbital shifts $V_i = U_i(1/2 - n_i)$ are adjusted to quasiparticle self-consistent GW (QSGW) calculations of the band structure, including the shifts of the band structure relative to the LDA one on an absolute scale. With this improved LDA+U model, good agreement is obtained for the minimum gap, the conduction band mass and the valence and conduction band shifts separately. The structural properties of ZnO also remain intact. When applied to the oxygen vacancy, we find the 2+/0 transition level in good agreement with recent hybrid functional calculations. Applications of the same LDA+U model to the Zn-vacancy are in progress and show that localization of the wave function on two oxygen neighbors is obtained.

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