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Quasi-particle self-consistent GW calculation of the band structure of β-Ga_2O_3[1] AMOL RATNAPARKHE, WALTER LAMBRECHT, Case Western Reserve University — β-Ga_2O_3 has recently received attention as an ultra wide band gap oxide. There are still uncertainties over its basic electronic structure. Here we present QSGW calculations of the band structure implemented in the linearized muffin-tin orbital approach. The QSGW approach usually overestimates the band gap, due to the underestimated screening in the random phase approximation (RPA) used to calculate W. Even after taking into account a universal 0.8 correction factor for this effect, we find a gap of order 5.4 eV, significantly higher than experimental values for the absorption onset. After inclusion of a lattice polarization effect on the screening, we find a minimum direct gap at Γ of 4.9 eV. The zero-point motion correction is estimated to be another 0.2 eV, leading to a final gap of 4.7 eV in good agreement with experiment. The indirect gap is found to be about 0.1 eV smaller. Symmetry labeling the states near the VBM and CBM at Γ shows that the lowest gap at Γ is allowed for $\mathbf{E} \perp \mathbf{b}$, and the first transition allowed for $\mathbf{E} \parallel \mathbf{b}$ occurs 0.6 eV higher. This predicted shift of the absorption onset for different directions is larger than found in experiment. Calculated absorption curves will be presented.

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