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Ab initio calculations of excitons in wurtzite-type semiconductors. NIELS E. CHRISTENSEN, University of Aarhus. DK-8000 Aarhus.., ROBERT LASKOWSKI, Technical University of Vienna, A-1060 Vienna — The optical absorption spectra are calculated with inclusion of electron-hole correlations for GaN, ZnO, and AlN, all in the wurtzite structure. Quasi-particle states are approximated by local-density-functional calculations with gaps corrected by a scissors operator, and the final spectra are obtained by solving the Bethe-Salpeter Equation . The results for ZnO depend sensitively on the energetic positions of the Zn-3d states. These are corrected by means of LDA+U. The excitons originating from the valence-band maximum are labeled A, B, and C, but their symmetry type, and thus dependence on the polarization of the light, are related to the specific values of the spin-orbit and crystal field splittings, SOC and CFS. The SOC is positive in GaN and AlN, negative in ZnO. The CFS is positive in GaN and ZnO, but negative in AlN. The sensitivity of the excitonic states to structural parameters is discussed, and in one case, AlN, we examine the validity of Elliott's model, the effective hydrogen-atom model.

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