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Band offsets at GaN/$ZnGeN_2$ interfaces ATCHARA PUNYA, WALTER LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, OH-44106-7079, USA — The interfaces of GaN/$ZnGeN_2$ are of interest because of their close lattice match and hence suitability of GaN as substrate for $ZnGeN_2$ film growth. In the present work, the band offsets for various polar and nonpolar interfaces between GaN and $ZnGeN_2$ are determined from full potential linear muffin-tin orbital (FP-LMTO) within the local density approximation (LDA). We determine the dipole potential formed at the interface from self-consistent supercell calculations and then add the difference between the bulk band-edges energy levels. Quasiparticle self-consistent GW corrections of the bulk band edges relative to the LDA edges are added. The strain state of the $ZnGeN_2$ is determined by assuming an unstrained GaN substrate with the $ZnGeN_2$ in-plane lattice constants matched to the substrate and the perpendicular lattice constant determined by minimizing the elastic strain energy using the known elastic constants. We find that the offset is type II, meaning staggered instead of straddled alignment, which is of interest for photovoltaic applications as holes and electrons would separate in different regions. The band offset depends slightly on interface direction. The orientation averaged valence band maximum of GaN is 0.86 eV lower than $ZnGeN_2$'s. The charge neutrality point alignment model is tested and found to give a significantly smaller band offset.

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