

Electronic Structure of ZnO:GaN Compounds: Asymmetric Bandgap Engineering

Muhammad N. Huda, Yanfa Yan, Su-Huai Wei, and Mowafak M. Al-Jassim

*National Renewable Energy Laboratory
Golden, Colorado 80401*

ZnO and GaN have a type-II band offset. The incorporation of one compound into the other would lead to a reduced bandgap as compared to that of either ZnO or GaN. Our density-functional theory calculation reveals an asymmetric bandgap reduction in this non-isovalent system, i.e., incorporating GaN in a ZnO host results in a much more effective bandgap reduction than incorporating ZnO in a GaN host. We further find that the random alloy system is more favorable than the superlattice system in terms of light absorption in the longer-wavelength regions. Our results suggest that the wavefunction localization at the band edges plays an important role in how to choose the host material and dopant for effective bandgap engineering through semiconductor compound alloying.