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**Material Properties of Widegap AlGaN for use in Power Electronics** NICHOLAS BALDONADO, New Mexico State University, JULIA DEITZ, Sandia National Laboratory, BORIS KIEFER, New Mexico State University — Materials with a significantly larger bandgap than silicon have emerged as a competing material platform for power electronics, including the development of light emitting UV diodes, materials with higher break-down voltages, and shorter switching times. Here we present results from parameter-free first principles density-functional-theory (DFT) computations on AlN, AlGaN, and GaN insulators and the effect of p- and n-doping on electronic, magnetic, and optical properties. Our computations benefit from the improved description of optical properties in materials using a self-consistent ACBN0 (Hubbard-U) approach. The preliminary results strongly suggest that both n- and p- dopants condense in proximity of defects such as surfaces, and interfaces. The detailed analysis of the associated electronic structure shows that the most stable surface truncations are metallic, changing the fundamental classification of these materials from insulating to conducting. We will discuss the effect of the predicted bandgap closure for applications of these materials in power electronics devices. Sandia National Laboratories are managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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