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New insights in the role of native defects in ZnO ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara CA 93106-5050 — ZnO is a wide-band-gap semiconductor with unique piezoelectric, optical, and electronic properties suitable for use in optoelectronic devices. The availability of bulk single crystals and a large exciton binding energy of 60 meV make ZnO a serious alternative to GaN. However, as-grown ZnO is nearly always n-type and the lack of reliable p-type doping still hinder its application for light-emitting devices. The unintentional n- type conductivity has been attributed to native defects, but the role of individual defects is still controversial. Here we investigate the electronic and structural properties of native defects in ZnO using Density Functional Theory within the Local Density Approximation. We will discuss methods for correcting the band-gap error inherent in density-functional theory. We explore the local atomic relaxations and their direct effect on the electronic structure of each native defect, diffusion barriers, and defect complexes. We will also report results for previously unexplored configurations. Finally, we discuss the influence of native defects on the control of p-type doping.

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