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### **Theory of defects and doping in ZnO<sup>1</sup>**

CHRIS G. VAN DE WALLE, University of California, Santa Barbara

In spite of rapid progress in materials quality, zinc oxide still suffers from serious problems in controlling its conductivity. We are addressing these issues by performing first-principles calculations based on density-functional theory (DFT) in the local density approximation (LDA). In addition, we have developed an approach (based on LDA+U) for overcoming the DFT band-gap problem, allowing us to more accurately compare and predict defect levels. Native point defects are still frequently invoked as sources of n-type conductivity, but our results do not support this hypothesis. Oxygen vacancies are deep donors; our configuration coordinate diagrams for this defect provide a detailed interpretation of the recent ODEPR results of Vlasenko and Watkins [1]. Zinc interstitials are shallow donors, but their formation energy is high and they diffuse very rapidly, with a migration barrier as low as 0.6 eV, making it very unlikely that they would be stable. For the zinc antisite, we find an unexpected low-symmetry configuration. While still high in energy, this defect may play a role under non-equilibrium conditions such as irradiation. We suggest that unintentional incorporation of impurities (such as hydrogen) is a more likely explanation for n-type background doping. However, native defects play a crucial role as compensating centers in p-type material, and we will discuss ways of overcoming this problem. Among the native defects that act as acceptors, zinc vacancies have the lowest formation energy; they introduce deep levels likely responsible for green luminescence. Our calculated migration barriers for the point defects are in good agreement with experimental data where available, and provide insight in the processes that take place during growth, irradiation, or annealing.

[1] L. S. Vlasenko and G. D. Watkins, Phys. Rev. B 71, 125210 (2005).

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