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Hybrid functional studies of defects and impurities in ZnO[1]

JOHN LYONS, University of California, Santa Barbara

Zinc oxide is regarded as a highly promising material for light-emitting diodes and lasers. Its features include a direct band gap of 3.4 eV, a large exciton binding energy of 60 meV, and the availability of high-quality single-crystal substrates. Despite the rapid development, fundamental issues regarding p-type doping remain unresolved. The most significant barrier to realizing ZnO-based optoelectronic devices is the difficulty in producing reliable and reproducible p-type material. Among the possible acceptor impurities, N has been considered the most promising because it has an atomic size close to that of O. In addition, N has been conclusively shown to act as a shallow acceptor in other II-V semiconductors, such as ZnSe. In spite of many published reports on p-type conductivity in N-doped ZnO, reproducibility and stability are still major issues, and devices based on $p-n$ homojunctions have remained elusive. In this work, we study the properties of the nitrogen acceptor using advanced density functional techniques. Our first principles calculations are based on hybrid functionals, which include a portion of exact exchange and correct the band gap of semiconductors, allowing us to accurately predict defect and impurity transition levels. Contrary to the conventional wisdom, we find the N acceptor has an exceedingly high ionization energy of 1.3 eV above the valence band, meaning that N cannot lead to hole conductivity in ZnO [1]. We have also analyzed the optical transitions (absorption and luminescence) and charge distribution associated with the N impurity, which offer characteristic signatures that can be compared to experimental results.

[1] J. L. Lyons, A. Janotti, and C. G. Van de Walle, APL **95**, 252105 (2009).

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