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How localized acceptors limit p-type conductivity in GaN[1]

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Despite the impressive development of GaN as an optoelectronic material, p-type conductivity is still limited. Only a single acceptor impurity, magnesium, is known to lead to p-type GaN. But Mg is far from a well-behaved acceptor. Hydrogen is known to passivate Mg, necessitating a post-growth anneal for acceptor activation. In addition, the ionization energy is quite large ($\sim$ 200 meV in GaN), meaning only a few percent of Mg acceptors are ionized at room temperature. Thus, hole conductivity is limited, and high concentrations of Mg are required to achieve moderately p-type GaN. Other acceptor impurities have not proven to be effective p-type dopants, for reasons that are still unresolved. Using advanced first-principles calculations based on a hybrid functional, we investigate the electrical and optical properties of the isolated Mg acceptor and its complexes with hydrogen in GaN, InN, and AlN.[2] We employ a technique that overcomes the band-gap-problem of traditional density functional theory, and allows for quantitative predictions of acceptor ionization energies and optical transition energies. Our results allow us to explain the deep or shallow nature of the Mg acceptor and its relation to the optical signals observed in Mg-doped GaN. We also revisit the properties of other group-II acceptors in GaN. We find that all cation-site acceptors show behavior similar to Mg_{Ga}, and lead to highly localized holes. The Zn_{Ga} and Be_{Ga} acceptors have ionization energies that are even larger than that of Mg, making them ineffective dopants. All acceptors cause large lattice distortions in their neutral charge state, in turn leading to deep, broad luminescence signals that can serve as a means of experimentally verifying the deep nature of these acceptors.

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[2]J. L. Lyons, A. Janotti, and C. G. Van de Walle, Phys. Rev. Lett. **108**, 156403 (2012).