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Shallow versus deep nature of Mg acceptors in nitride semiconductors[1] JOHN LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Although Mg doping is the only known method for achieving p-type conductivity in nitride semiconductors, Mg is not a perfect acceptor. Hydrogen is known to passivate the Mg acceptor, necessitating a post-growth anneal for acceptor activation. Furthermore, the acceptor ionization energy of Mg is relatively large (200 meV) in GaN, thus only a few percent of Mg acceptors are ionized at room temperature. Surprisingly, despite the importance of this impurity, open questions remain regarding the nature of the acceptor. Optical and magnetic resonance measurements on Mg-doped GaN indicate intriguing and complex behavior that depends on the growth, doping level, and thermal treatment of the samples. Motivated by these studies, we have revisited this topic by performing 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. With the help of these advanced techniques we explain the deep or shallow nature of the Mg acceptor and its relation to optical signals often seen in Mg-doped GaN. We also explore the properties of the Mg acceptor in InN and AlN, allowing predictions of the behavior of the Mg dopant in ternary nitride alloys.

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[X] Prefer Oral Session
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