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Stability and electronic structure of Mg dopants in InGaN alloys

JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Nitride semiconductors have attracted much attention due to their applications for light emitting and laser diodes. High conductivity p-type nitride layers are demanding for various optoelectronic devices, however, hole concentrations are generally low because of the deep acceptor level of Mg and the compensation of hole carriers by donor defects. In this work, we investigate the stability and electronic properties of Mg dopants in InGaN alloys through first-principles density functional calculations. We generate the alloy structure with the In content of 10% by using the special quasi-random structure approach. Considering various Mg sites surrounded with different numbers of the In atoms in the second nearest neighborhood, we find that Mg dopants prefer to be located near the Ga atoms rather than the In atoms due to the local bonding effect. Incorporation of the In atoms not only reduces the band gap but also decreases the ionization energy of Mg in Ga-rich regions. However, the ionization energy tends to increase as the number of the In atoms in the second nearest neighborhood increases, although this configuration is energetically unfavorable.

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