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Stability of oxygen dopants in group-III nitride alloys JI-SANG PARK, National Renewable Energy Laboratory, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — Group-III nitride materials have attracted much attention for their potential applications in light-emitting devices such as light-emitting and laser diodes. Low resistivity p-type layers are demanding, however, the p-type doping efficiency is still low due to high Mg acceptor level and compensating donor defects such as interstitial hydrogen and nitrogen vacancy. Several donor-acceptor co-doping methods have been suggested to enhance the p-type doping efficiency in group-III nitrides; however, there is a lack of study on the stability and electronic properties of donor dopants in nitride alloys. In this study, we investigate site preference of oxygen dopants in group-III nitride alloys including ternary AlGaN and quaternary AlInGaN alloys through first-principles density functional calculations. We adjust the composition ratio of Al and In to make the band gap of AlInGaN same to that of AlGaN. In AlGaN, we find that the oxygen dopants tend to bond with Al atoms due to the high bond energy between Al and O. The same tendency is found in AlInGaN, whereas the dopants also become stable as they are bonded to In atoms due to small strain.

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