Efficient luminescent center by codoping of (Eu, Mg, O) to GaN

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Graduate School of Engineering, Osaka University — From a theoretical point of view, we propose that GaN codoped with Eu, Mg, and O is a good photoluminescent material. We guess that codoping of O besides Eu and Mg to GaN can promote the recombination of excitons, where the compound of Eu and Mg codoped GaN has been already reported with high validity of light emitting in experiments. [1] In this work, we used the Vienna ab-initio simulation package (VASP). [2] As a result, we found that the three impurity elements tend to assemble themselves energetically in the host crystal GaN, though the two elements (Eu and Mg) do not. Moreover, the complexes of Eu-O-Mg generate an area with a band gap that is narrower than the host crystal. This means that the complexes can attract and trap excitons that are generated around the complexes. Consequently, most of excitons must recombine there and convert into light efficiently. [1] D. Lee, A. Nishiwaka, Y. Terai, et al., Appl. Phys. Lett. 100 (2012) 171904. [2] G. Kresse and D. Joubert, Phys. Rev. B 59 (1999) 1758.