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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.

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