# First-principle investigation on electron induced hydrogen migration in Eu/Mg co-doped GaN

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Mg doped GaN is a promising for high efficient nitride-based light emitting diode. However, the presence of hydrogen has limited its efficiency by electrical passivation of p-type Mg acceptors. Experimental study shows that the p-type conductivity recovers under low energy electron beam irradiation (LEEBI) treatment. The improved p-type conductivity is often attributed to dissociation of neutral Mg-H complexes. However, previous studies on dissociation kinetics of Mg doped GaN utilizing photoluminescence showed strong dependencies on growth method and environmental conditions as well as thermal history of the sample and thus none of study has provided a final clear understanding on the improved excitation efficiency in Mg doped GaN after LEEBI treatment. Moreover, generation of new excitation channels made it difficult to distinguish the luminescence originated from different energy levels and made no suggestion on atomistic origin. Additional Eu doping opens a new avenue to probe the atomic scale behavior of hydrogen-related complexes by using sensitivity of the Eu center emission [1]. In this study, first-principle density functional theory (DFT) is employed to understand the change in luminescence under electron beam irradiation. The comparison on energetics of three different Eu/Mg cluster configurations and change in Eu emission of Eu/Mg co-doped GaN has provided the atomistic origin of enhanced luminescence [2].

Figure 1(a) shows the energetically favorable Eu-H-N-Mg-Vacancy cluster configuration (Eu/Mg1) obtained from our DFT calculations. With an excess electron, however, the Eu/Mg1 is energetically less favorable and another configuration, which hydrogen sits on the vacancy site (Eu/Mg2), becomes energetically more preferred, see Fig. 1(b). In addition, a slightly different configuration, in which hydrogen migrates to the opposite interstitial site from the Eu ion (Eu/Mg3) become energetically equally stable with the Eu/Mg1, see Fig. 1(c). Additional excess electrons further increases the stability of Eu/Mg2 and Eu/Mg3 configuration, while decreases the stability of Eu/Mg1. Table1 summarizes the change in energetics of three different configurations and atomic displacement of Eu ion with respect to un-doped Eu:GaN. These results resemble well the experimentally observed instability of the Eu-Mg centers under LEEBI treatment.

## Conclusion

DFT calculations demonstrate that the migration of hydrogen relative to the Mg in Eu/Mg centers can well describe the observed behavior of these centers under e-beam irradiation. Moreover, since the DFT calculations also predict similar energetic changes associated with hydrogen migration for complexes without the Eu ion, we demonstrate that the use of Eu ions as a probe has a potential to shed more inside into the dynamics of acceptor activation in Mg-doped p-type GaN.

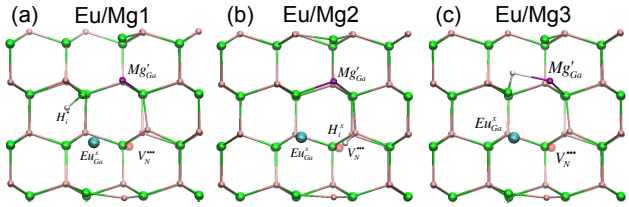


Figure 1. Three different Eu-H-N-Mg-Vacancy configuration obtained from DFT calculation. While Eu/Mg1 is the most energetically favorable in neutral state, Eu/Mg2 become energetically more stable with excess electrons. Metastable Eu/Mg3 is also becoming more stable than Eu/Mg1 with excess electrons.

Table I. Comparison on relative energetics among Eu/Mg1, Eu/Mg2, Eu/Mg3 configurations without and with one and two excess electrons. The atomic displacements of $Eu_{Ga}^{x}$ with respect to the position in the undoped Eu:GaN are also compared

| | Relative energy (eV) | | | Atomic displacement (Å) |
|---|---|---|---|---|
| | No electron | One electron | Two electron | |
| Eu/Mg1 | 0 | 0.17 | 0.83 | 0.319 |
| Eu/Mg2 | 0.96 | 0 | 0 | 0.065 |
| Eu/Mg3 | 0.12 | 0.17 | 0.61 | 0.003 |

## Open Questions

1. Will the Mg-doped GaN show similar energetics for the dissociation of Mg-H complex without presence of Eu ion after LEBBI treatment?
2. What is the mechanism for the improved p-type conductivity and light emitting efficiency from the rearrangement of the Mg-H defect complex?
3. How can we control the dissociation kinetics to achieve the desired properties of GaN?

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