Magnetism in Eu Doped GaN bulk and nanoparticles: Effects of Si codoping

Vijay Kumar

Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon, Haryana 122 001, India and Center for Informatics,

School of Natural Sciences, Shiv Nadar University, Chithera, Gautam Budh Nagar, Uttar Pradesh 203 207, India

1. Introduction

GaN doped with rare earths such as Eu, Er, and Tm has been widely studied [1] experimentally to produce bright luminescence in visible range. However, theoretical studies are few [2,3]. Eu doping in GaN produces luminescence in red region (621 nm). It has been found that co-doping with Si enhances luminescence by 5-10 times due to the increase in the PL lifetime. However, increasing the Si contents decreases the luminescence. Since Si is tetravalent, it is expected to behave as an intrinsic donor when co-doped with Eu in GaN.

2. Method of calculation and results

We have studied [3] substitutional doping of Eu (1-2%) on Ga site and also co-doping of Si on Ga site using *ab initio* projector augmented wave pseudopotential method and 3x3x3 supercell with 108 atoms (Fig. 1). We treat all the f electrons on Eu as valence electrons and therefore also study the magnetic properties. It has been found that Eu on a Ga site lowers the local symmetry but it is energetically unfavorable. It has 6 μ_B magnetic moments. Addition of Si makes Eu doping energetically favorable and the f levels of Eu become half-filled with 7 μ_B magnetic moments. Within GGA the up-spin f levels of Eu lie at the top of the valence band with a hole. As f electrons are very localized, we also considered the effects of on-site Coulomb interactions. This shifts the up-spin f levels downwards, makes them hybridize with the valence band and become quite spread (see Fig. 1). However, Si co-doping shifts the f levels in the band gap of GaN with a sharp peak (Fig. 1). This could explain the long life of excitations with Si doping. Also doping of 2 Eu atoms with and without Si atom has been studied (Fig. 1) and the magnetic coupling between Eu atoms has been explored.

Further calculations have been performed [4] on GaN small nanoparticles that favor an empty cage structure. Doping of these cages with Eu as well as Si, show behavior similar to bulk but energetically it is better to dope Eu in nanoparticles. In nanoparticles there are different Ga sites where doping can be done. We have studied doping at different sites and obtained the most favorable configuration. Similar to bulk, the magnetic moments in nanoparticles are 6 and 7 μ_B without and with Si doping, respectively. Nanoparticles could offer a good possibility to make Eu doping easier than in bulk and the reduced symmetry in nanoparticles could offer better probability of *f-f* transition. Preliminary results of Eu doping will also be presented in thin slabs with wurtzite structure. On the other hand few layers of GaN become planar with graphitic structure when fully optimized [5].
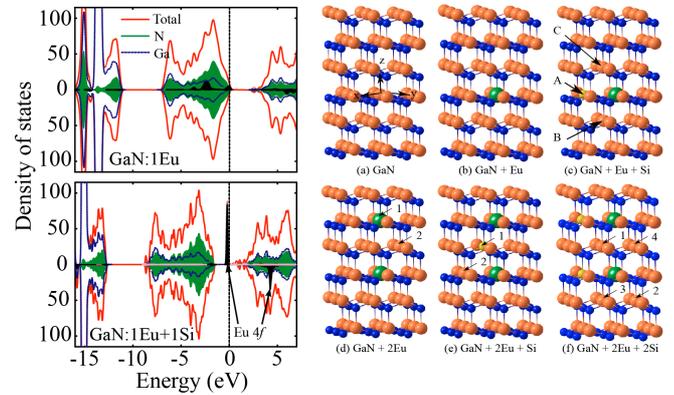
3. Conclusions

Fig. 1. Atomic structure of 3x3x3 supercell of pure as well as doped GaN. 1, 2, 3 … show the sites that have been studied for doping. Pink, blue, green, and yellow balls show Ga, N, Eu, and Si atoms, respectively. The total and partial densities of states have been shown using GGA+U method. Zero of energy is the Fermi energy.

Co-doping of Si is energetically better and leads to a further reduction in the local symmetry around Eu ion. In the presence of Si, Eu behaves as a divalent specie with 7 μ_B magnetic moment that are ferromagnetically coupled. Nanoparticles could offer a better way to dope Eu.

4. Open questions

(1) The effects of defects and temperature need to be understood. (2) Proper treatment of band gap is needed.

References

[1] S. J. Peaton, U. Hommerich, J. T. Seo, R. G. Wilson and J. M. Zavada., Appl. Phys. Lett. **72**, 2710 (1998).
[2] A. Svane, N. E. Christensen, L. Petit, Z. Szotek and W. M. Temmerman., Phys. Rev. B. **74**, 165204 (2006).
[3] A. Vallan Bruno Cruz, P. P. Shinde, V. Kumar, and J.M. Zavada, Phys. Rev. B**85**, 045203 (2012).
[4] P. Kaur, S.S. Sekhon, and V. Kumar, Phys. Rev. B **85**, 085429 (2012) and to be published; P. Kaur, S.S. Sekhon, J.M. zavada, and V. Kumar, to be published.
[5] P. Kaur, P.P. Shinde, S.S. Sekhon, and V. Kumar, to be published.