Electronic and Magnetic Properties of Eu doped GaN nanowires: An Ab-initio study for spin-optoelectronic applications

V. K. Gudelli[#] and I. S. Roqan[*]
Physical Sciences and Engineering Division, King Abdullah University of Science and Technology, Thuwal-23955-6900, Saudi Arabia
[#]Presenting author *Corresponding author e-mail: iman.roqan@kaust.edu.sa

Abstract Submission

The properties of Eu-doped GaN nanowires (NWs) grown along the wurtzite orientation are calculated using density functional theory (DFT) based on the generalized gradient approximation (GGA) including the Hubbard (U) parameter. Our simulation reveals that Eu impurities (Eu_s) prefer to locate on the NW surface, while they are more stable than the native point defects. Further increase in the Eu density, opens the lattice, thus reducing the energy of the formation of point defects. The density of states (DOS) shows the Eu impurities state in the NWs bandgap, which can be the factor responsible for interesting optical, electrical, and magnetic properties of Eu-doped GaNNWs. The unique magnetic properties are revealed, indicating in-plane and out-of-plane magnetic anisotropy energy (MAE), depending on Eu_s- defect configuration.

Introduction

The nanostructure of rare earth (RE) doped wide band gap nitrides are of interest in optoelectronic applications, such as in visible lasers due to the 4f partial transition states, resulting in sharp emission that is not affected by temperature. GaN doped with RE impurities has attracted many researchers. Eu-doped GaN is fascinating due to its potential magnetic and optical properties [1]. However, the mechanism behind the magnetic behaviour of Eu in GaN NWs is not well investigated in the literature

Model

VASP is used to carry out the computations. The projected augmented wave (PAW) basis set with GGA in the Perdew-Burke-Ernzerhof (PBE) form is used to describe the exchange and correlation effects [2] along with the GGA+*U* method. The on-site Coulomb parameter *U*=6.7eV with a *J* value of 0.7eV is used for Ga, and *U*=7.4eV with a *J* value of 1.109eV is used for Eu.

Results and Discussion

We see that the Eu atom is a stable defect as indicated by the negative formation energy values. The total and projected density of states of the NWs are calculated with Eu dopant along with point defects and is presented in Fig. 1 and 2. The DOS indicates that the Eu *f*-states is located in the band gap of GaN NWs, activating impurity states, while the valence band maximum (VBM) moves towards/away from the Fermi-level in presence of N and Ga vacancies (V_N and V_{Ga}). The calculated magnetic moment of Eu-doped GaN NWs increases in the presence of the N and Ga vacancies. Further, as the density of Eu impurity increases in NWs with intrinsic defects leads to out-of-plane magnetic anisotropy energy (MAE) for all Eu-intrinsic defect doped GaNNW configurations apart from Eu-V_{Ga}, which shows in-plane MAE. The out-of-plane MAE is found to increase with the increase in the number of Eu atoms in NWs this could have valuable applications in high-density data storage devices.

Conclusion

The intra-band *f-f* transitions from the electronic structure calculations and higher value MAE makes the Eu-doped GaN nanowires a favourable candidate for optoelectronic and data storage device applications.

Acknowledgment

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References

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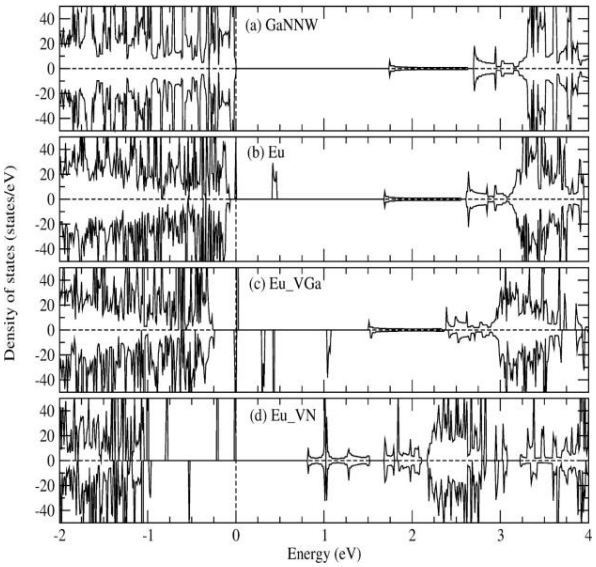

Fig. 1. The Density of states of GaN NW with Eu doping and point defects.

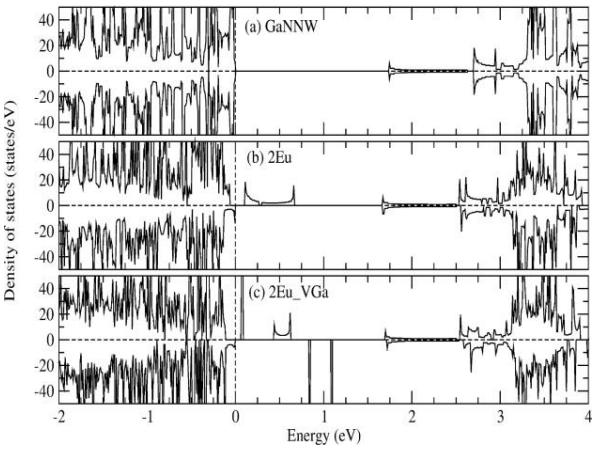

Fig. 2. The Density of states of GaN NW with 2Eu doping and point defects.

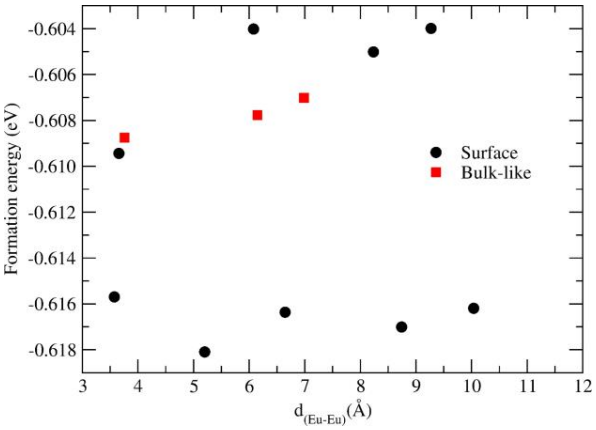

Fig. 3. The formation energy of Eu-doped GaN NW with the variation of Eu distance in NW.