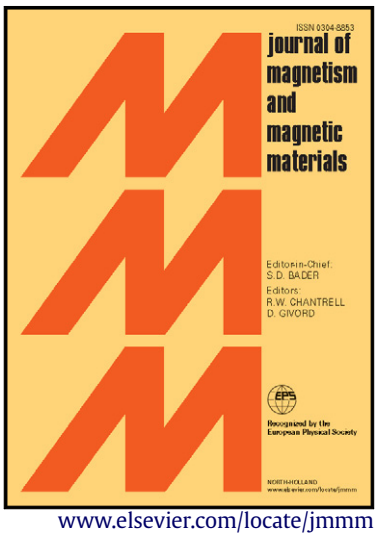

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A Density Functional Theory Study of 3d and 4f exchange interactions in Cr-Nd co-doped GaN

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The density functional theory based calculations of Cr, Nd and Cr/Nd co-doped wurtzite GaN generated using GGA and TB-mBJ exchange correlation functionals are being reported. All the structures were geometrically optimized and fully relaxed. The dopants introduced new energy levels in the forbidden energy gap, whose hybridization and interaction are discussed in detail to explain electronic and ferromagnetic properties of the materials. The 3d-3d interaction seems to be responsible for double exchange interaction in Cr:GaN whereas spin polarization caused by 4f-5d-CB interaction causes ferromagnetism in Nd:GaN. A model is proposed to explain the ferromagnetic ordering in new co-doped system Cr/Nd:GaN according to which 4f-5d-CB-3d interaction via 4f-5d, 4f-2p and 2p-3d coupling plays role.

HIGHLIGHTS

1. DFT study of Cr-Nd codoped GaN
2. Double Exchange interaction in Cr:GaN
3. 4f-5d-CB exchange interaction in Nd:GaN
4. 4f-5d-CB-3d exchange interaction in Nd/Cr:GaN

Keywords

Density Functional Theory: GaN; Co-doping; TM; RE; GGA; TB-mBJ