

Abstract Submitted  
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**Ferromagnetism in Mn doped GaN Nanowires** QIANG SUN, QIAN WANG, PURU JENA, VCU — Using density functional theory and generalized gradient approximation for exchange and correlation potential we show that the magnetic coupling of Mn atoms in the nanowires, unlike that in the thin film, is ferromagnetic in spite of the thickness of the wire and the contraction of the Mn-Mn and Mn-N bond distances. This ferromagnetic coupling, brought about due to the confinement of electrons in the radial direction and the curvature of the Mn-doped GaN nanowires' surface, is mediated by N as is evidenced from the overlap between Mn  $3d$  and N  $2p$  states. The Mn atoms prefer to occupy the nearest neighbor positions on the outer surface of the wire and carry a magnetic moment ranging from 0.56 to 3.5  $\mu_B$ /atom depending on the thickness of the wire. Calculations of the anisotropic energy show that the magnetic moment orients preferably along the  $[10\bar{1}0]$  direction while the wire axis points along the  $[0001]$  direction. The flexibility of both controlling the magnetic coupling and the magnetic moment by choosing the dimensionality and the size of the wire may be useful in practical applications. The results are in agreement with the recent experimental data which show that Mn-doped GaN nanowire can be ferromagnetic without the presence of other defects.

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