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Embedded Clustering and Metastable Magnetism in Transition-Metal doped III-Nitrides[1] CUI XIANGYUAN, The University of Sydney, JULIA MEDVEDEVA, University of Missouri-Rolla, ARTHUR J. FREEMAN, Northwestern University, BERNARD DELLEY, Paul-Scherrer-Institut, CATHERINE STAMPFL, The University of Sydney — From extensive density-functional theory calculations [1] we find that Cr atoms in GaN prefer to form embedded clusters, occupying Ga sites [2]. Significantly, for larger than 2-Cr- atom clusters, states containing antiferromagnetic coupling with net spin in the range 0.06-1.47 μ_B/Cr are favored. Similar behavior is found for Mn:GaN, and Cr:AlN and Mn:AlN. We show that various configurations may coexist leading to a strong dependence of the magnetic properties on the growth conditions. This elucidates many puzzling observations such as the 5 (20-30) times lower value of the measured magnetic moment on Cr (Mn) as compared to the theoretically predicted one for the isolated dopants. In addition to the expected ground high spin (HS) states for isolated Mn and Fe in GaN (4 μ_B/Mn and 5 μ_B/Fe), metastable low spin (LS) states (0 μ_B/Mn and 1 μ_B/Fe) are found. The transition between the HS and LS states corresponds to an intra-ionic electron transfer between the t_2 and e orbitals, accompanied by a spin-flip process.

[1] B. Delley, J. Jchem. Phys. **113**, 7756 (2000).
[2] X.Y. Cui, *et al.*, Phys. Rev. Lett. Dec. 2005.

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