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First Principles Investigation on the Spatial Distribution and Magnetism in Cr doped GaN X.Y. CUI, C. STAMPFL, School of Physics, The University of Sydney, Sydney 2006, Australia, B. DELLEY, Paul Scherrer Institut WHGA/123 CH-5232 Villigen PSI, Switzerland, J MEDVEDEVA, A.J. FREEMAN, Department of Physics & Astronomy, Northwestern University, Evanston, Illinois 60208 — Exhaustive structural and magnetic configurations have been investigated to understand the magnetism of Cr:GaN. Our results provide direct evidence that the magnetic ions have a strong tendency to get close by forming "constrained clusters" with short-range magnetic interactions. Substitutional clustering configurations are found much more favourable than the substitutional-interstitial complexes. Significantly, while for isolated and "pair" substitutional configurations the ferromagnetic state is the ground state with a magnetic moment close to $3\mu_B$/Cr, for more than three Cr atoms configurations, antiferromagnetic states are found energetically more favourable where the net spin is much lower (0-1.8 μ_B). We propose a picture that various Cr-configurations coexist and the statistical distribution and associated magnetism depend sensitively on the growth conditions. Such a view can elucidate and explain many of the hitherto puzzling experimental observations. We argue such a picture may also hold for other diluted magnetic semiconductor systems.

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