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Antiferromagnetic coupling driven by bond length contraction near $Ga_{1-x}Mn_xN$ film surface WANG QIAN, QIANG SUN, PURU JENA, Virginia Commonwealth University, YOSHI KAWAZOE, Tohoku University — Following the discovery of ferromagnetism in (Ga,Mn)As and the subsequent theoretical prediction that Mn doped GaN could be ferromagnetic at or above room temperature, numerous attempts have been made to synthesize this promising DMS material. However, the results have been rather confusing. Not only the reported Curie temperatures vary over a wide range (10K-945K), but also it is uncertain whether the ground state of (Ga,Mn)N is ferromagnetic (FM) or antiferromagnetic (AF). An understanding of the controversy between FM and AF is both important and challenging. Using first principles calculations based on gradient corrected density functional theory we show that Mn atoms, which couple ferromagnetically in bulk $Ga_{1-x}Mn_xN$, couple antiferromagnetically on its surface. This change in magnetic behavior is brought about a contraction of the Mn-Mn and Mn-N bond lengths which is significantly smaller on the surface than in the bulk. The present study provides new insight for explaining the numerous conflicting experimental observations in Mn doped GaN systems.

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