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Nitrogen defects and ferromagnetism in Cr-doped AlN BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — It is believed that N defects play important roles in achieving high-temperature ferromagnetism in Cr-doped AlN. We use state-of-the-arts DFT method to investigate N defects and their effects on ferromagnetism of (Al,Cr)N with N vacancies V_N. Our total-energy calculations show that the nearest Cr-Cr pair with the two spins in parallel is the most favorable and the nearest Cr-V_N pair makes a stable complex. Our formation energies indicate that V_N regions can be formed spontaneously under N-poor condition, or Cr-doped regions can be formed under N-rich condition. Hence real samples should be inhomogeneous. Both of the single Cr and V_N create filled electronic states in the semiconductor gap of AlN. N vacancies enhance the ferromagnetism by enlarging Cr moment, but reduce the ferromagnetic exchange constants between the spins in the nearest Cr-Cr pairs. These calculated results are in agreement with experimental observations and facts. Phys. Rev. B 78, 195206 (2008).

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