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Electronic structure and ferromagnetism of Mn δ-doped GaN
JOONGOO KANG, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea — Recently, Mn-doped GaN has attracted much attention because of the ferromagnetism observed in this material. However, experimental data so far are quite controversial, reporting the Curie temperatures ranging from 10 to 940 K. Very recent experiments showed that Mn δ-doped GaN films have high hole carrier concentrations, which lead to the high Curie temperature and enhanced magnetization. In this work, we study the electronic and magnetic properties of Mn doped GaN and the origin of p-type conductance especially for Mn δ-doped films through first-principles spin-density-functional calculations. The nature of magnetic interactions between two Mn ions is investigated by varying the Mn-Mn distance and their orientation. The ferromagnetic coupling has a short-range nature, effective for Mn-Mn distances up to about 7 Å. We also investigate the doping effect on ferromagnetism, and the energetics and ferromagnetism of Mn nanoclusters. Finally, we find that Ga vacancies near the Mn δ-doped layer are more stable than in the bulk region of GaN due to the charge transfer from the Mn to Ga vacancy. We suggest that Ga vacancies near the Mn δ-doped layer are likely to be the origin of p-type conductance.

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