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Intrinsic spin polarization of cation vacancies in group-III nitrides
YOSHIHIRO GOHDA, Department of Physics, The University of Tokyo, 113-0033, Japan, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo, 113-8656, Japan — Group-III nitrides are of significant importance not only in optoelectronic devices but also in potential applications to spintronics. Recently, we have clarified by means of total-energy DFT+U calculations that spins of Ga vacancies in Gd-doped GaN interact ferromagnetically [1]. We have also found that the magnetic moment increases monotonically with the increasing number of Ga vacancies, which explains experimental observations of colossal magnetic moments in Gd-doped GaN [2]. In this contribution, we report newly performed first-principles calculations that clarify spin polarization and lattice relaxation of cation vacancies with various charge states in a few group-III nitrides. Spin-polarized electronic configurations obtained in the present study are indicative of intrinsic ferromagnetism due to cation vacancies in nitride semiconductors.
[1] Y. Gohda and A. Oshiyama, Phys. Rev. B 78, 161201 (R) (2008).
[2] S. Dhar et al., Phys. Rev. Lett. 94, 037205 (2005).

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