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Spin-Based Strain Sensing in Two-Dimensional GaN: An Ab Initio Investigation of Magnetic Defects.

The development of nanoscale sensors capable of detecting mechanical strain through spin-dependent responses represents a promising approach to emerging sensing technologies. In this context, gallium vacancies in two-dimensional gallium nitride (GaN) can induce localized magnetic centers whose electronic and magnetic properties may be tuned by mechanical strain[1}.

In this work, the potential of these defects for strain sensing is investigated through first-principles calculations based on density functional theory (DFT), using VASP within the GGA-PBE approximation and the projector augmented-wave (PAW) method. Different spin configurations were evaluated, and the electronic and magnetic properties were characterized through band structures, projected densities of states, and spin density distributions.

The results reveal a total magnetic moment of 3 μB, with magnetization primarily localized in the p orbitals of the nitrogen atoms neighboring the vacancy. The spin–spin contribution to the zero-field splitting (ZFS) exhibits axial character, with parameters $D = -2.486$ GHz and $E \approx 0$. Its modulation under biaxial strain is currently being investigated to establish a sensing mechanism based on shifts in spin transition frequencies.

1] M. You, C. He, G. Guo, C. Zhang, and J. Zhong, Phys. Rev. B 113, 054113 (2026).
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