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

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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.

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.