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Structure dependent electronic and magnetic properties of graphitic GaN-ZnO nanoribbons

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1. The electron coupling and local magnetic moment

Considering only two coordinate edge N and Ga atoms (with a dangling bond) have unpaired electrons, we used two unit cells to simulate the ferromagnetic, ferromagnetic and antiferromagnetic coupling of the electrons (as shown in Figure S1 and Table S1). The two coordinate edge N and Ga atoms (N1, N2, Ga1, Ga2) are shown in Figure S1, and the arrangements of unpaired electrons are shown in Table S1. The results indicate that the ferromagnetic coupling of the electrons is the most favorable case (with the lowest energy). The two types of ferrimagnetic coupling structures (Ferrimagnetic1 and Ferrimagnetic2 with a spin down electron at N or Ga atom respectively as shown in Table S1) are not stable, which would tend to become antiferromagnetic and ferromagnetic coupling structures respectively.

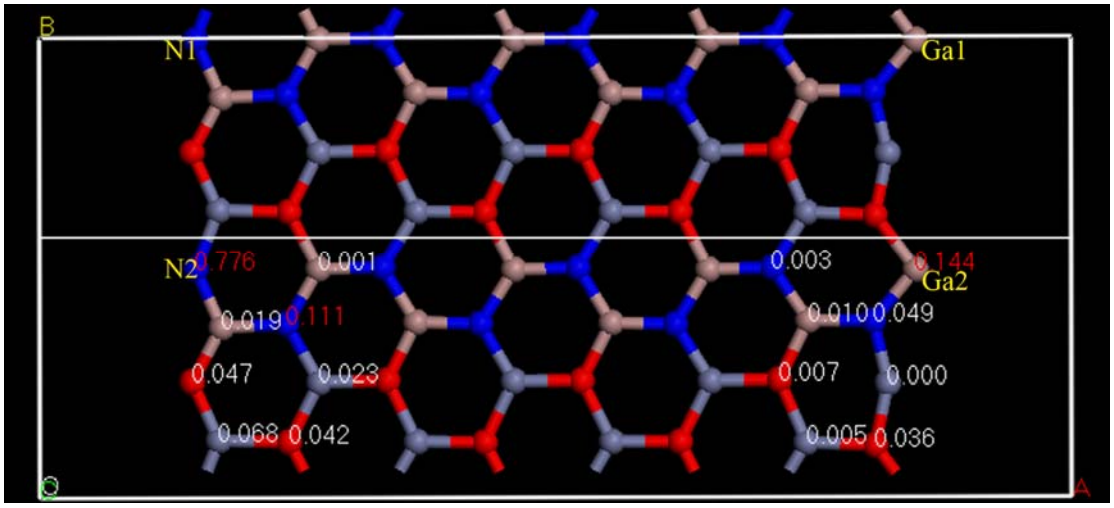

Figure S1. The local magnetic moments at edge and near edge atoms for ferromagnetic coupling case.

The local magnetic moments at edge and near edge atoms (for ferromagnetic coupling case) are shown in Figure S1 (the magnetic moments in one unit are shown and that of another are the same). We can see that the unpaired spin is mainly originated from the unsaturated edge atoms (due to the dangling bonds at the edges), and the inner atoms close to the edges also contribute a small amount of unpaired spin (due to the delocalization of the electrons). The most contributed atoms are edge N atoms (0.776 μ_B/atom) which followed by edge Ga atoms (0.144 μ_B/atom) and near edge N atoms (0.111 μ_B/atom).

Table S1. Energy difference (Δ E) and total magnetic moments (M) of ferromagnetic, ferromagnetic and antiferromagnetic coupling systems (+1 denotes spin up and -1 denotes spin down).

	N1	N2	Ga1	Ga2	M(μ_B)	△E(meV)
Ferromagnetic	+1	+1	+1	+1	4.00	0
Antimagnetic	+1	-1	+1	-1	-0.46	4
Ferrimagnetic1	-1	+1	+1	+1	-0.16	189
Ferrimagnetic2	+1	+1	-1	+1	4.00	0