First-principles investigations of zigzag GaN nanoribbon via symmetric/asymmetric edge functionalization

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Abstract
Density functional theory (DFT) is used to investigate the structural, electronic, magnetic, and transport properties of zigzag GaN nanoribbons (ZGaNNRs) with symmetric and asymmetric edge functionalizations. We have also investigated the performance analysis of nanoscale interconnect circuits based on the considered structures. All passivated topologies of sp^2 and sp^3 exhibit thermodynamic stability and exothermic characteristics, demonstrating the viability of chemical edge engineering. The asymmetric F-ZGaNNR-FH (Ga edge is functionalized with F atom and N edge is functionalized with F and H atoms) configuration is the most energetically favorable among all the structures examined. It has a binding energy of 5.71 eV at width (Nz) = 8. As the F atom concentration increases, the Fermi level shifts downward systematically, leading to strong p-type doping. Localized edge states provide strong magnetism in all functionalized nanoribbons. Each system stabilizes in the antiferromagnetic ground state, and the magnetic energy differences are greater than thermal excitations at ambient temperature. In group-C nanoribbons, half-metallic behavior emerges when hydrogen atoms terminate the N-edge, whereas fluorine passivation results in metallic character in both spin channels. Quantum transport calculations also show significant negative differential resistance (NDR) characteristics. Notably, fully hydrogen-passivated nanoribbons from all groups exhibit the highest peak-to-valley ratios: 84.19%, 92.85%, and 89.26%, respectively. These findings indicate that edge functionalization offers an effective method to tailor ZGaNNRs for future spintronic and nanoelectronics applications.

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