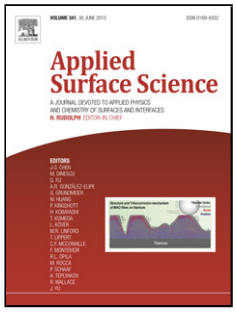

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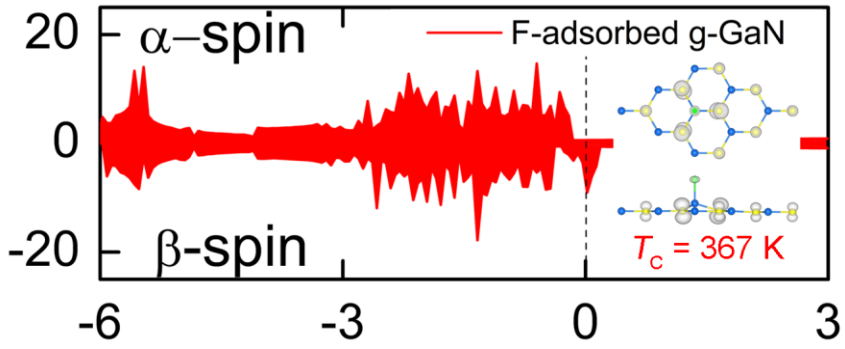
Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers

Wencheng Tang,[*a] Minglei Sun,[a] Jin Yu,[b] Jyh-Pin Chou[c]

[a]*School of Mechanical Engineering, Southeast University, Nanjing, Jiangsu 211189,China*
[b]*School of Materials Science and Engineering, Southeast University, Nanjing, Jiangsu 211189, China*
[c]*Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, POB 49, Hungary*

[*)] Author to whom correspondence should be addressed. Electronic mail: 101000185@seu.edu.cn

Graphical abstract



Highlights

1. Magnetic states are founded in B-, C-, N-, and F-adsorbed g-GaN monolayers.
2. A spin-polarized semiconducting state appears in the B- and C-adsorbed g-GaN systems.
3. A half-metallic state appears in the N- and F-adsorbed g-GaN systems.
4. The F-adsorbed system that exhibits a high Curie temperature of 367 K.

Abstract

The electronic and magnetic properties of graphene-like gallium nitride (g-GaN) with adsorbed H, B, C, N, O, and F atoms were investigated using spin-polarized first-principles calculations. We found that H, B, C, N, O, and F atoms can be chemisorbed on a g-GaN monolayer. The total magnetic moments of 1.0, 2.0, 1.0, and 1.0 μ_B are founded in B-, C-, N-, and F-adsorbed g-GaN monolayers, respectively. In addition, a half-metallic state appears in the N- and F-adsorbed g-GaN, while a spin-polarized semiconducting state appears in other g-GaN monolayers after the adsorption of B or C. These findings demonstrate that the magnetic properties of g-GaN can be effectively tuned by