Introducing robust magnetism in boron-doped graphene nanoribbons with non-benzenoid defects

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Although recent studies have reported the existence of high spin states on free-standing 7-armchair graphene nanoribbons (7-AGNR) with topological defects [1] and boron-doped nanoribbons (7-BGNR) [2], the magnetism is not robust enough to endure on a gold substrate. In contrast, previous studies on carbon-based triangulene dimers and hexamer nanostars have shown that the magnetic character of adsorbed species is not totally screened by the Au(111) substrate and magnetism persists [3-4]. With the help of first-principles DFT+U calculations, we propose to address the issue associated with weak magnetism in GNRs by incorporating non-benzenoid pentagon defects in 7-BGNRs. The presence of such defects strengthens its exchange coupling energy, for both free-standing and Au(111) adsorbed species. Our results show that the pentagonal defects in pristine 7-AGNR leads to antiferromagnetic (AFM) free-standing ground state; while on Au(111) surface, it becomes ferromagnetic (FM) with a triplet spin configuration (Fig. 1). This variation mostly originates from the p-type doping nature of the substrate. Contrarily, pentagonal defects in 7-BGNR gives relatively stable FM ground state for both free-standing and adsorbed phases on Au(111). In addition, we have found that the magnetism is strongly localized nearby the non-benzenoid defect sites of the 7-AGNR, even on the Au(111) surface. In summary, our study provides new insights into the design of magnetic graphene-based systems, and suggests a promising approach for tailoring their magnetic properties.

References

[1] D. J. Rizzo et al., *Science*, *369*(6511) (2020) 1597-1603.
[2] N. Friedrich et al., *Phys. Rev. Lett.*, *125*(14) (2020) 146801.
[3] S. Mishra et al., Angew. Chem. Int. Ed., 59(29) (2020) 12041-12047.
[4] J. Hieulle et al., Angew. Chem. Int. Ed., 60(48) (2021) 25224–25229.

Figures

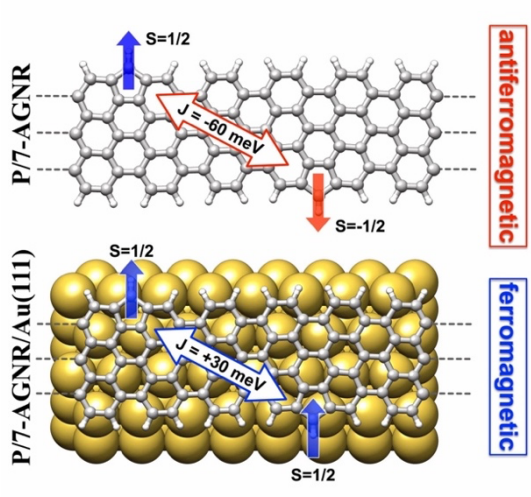

Figure 1: Non-benzenoid pentagon defects in 7-AGNR backbone introduces open-shell singlet state in free-standing phase while a FM triplet state is observed when adsorbed on Au(111) surface.