Graphene Nanoribbons with a magnetic Edge

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Introduction

Traditional magnetic materials are based on the transition metals such as Fe, Co and Ni, whose magnetic ordering originates from the partially filled *d*-electron bands. Metal-free carbon structures exhibiting magnetic ordering represent a new class of materials and open a novel field of research. The successful isolation and epitaxial growth of graphene, in particular, have stimulated extensive experimental and theoretical work on the magnetic properties of graphene nanoribbons, nanoflakes and defects. The driving force behind these studies was not only for their many technological applications, but also for their fundamental scientific interest. The central problem is to understand the origin of magnetism in a system which contains only *s*- and *p*-electrons and has traditionally been thought to show diamagnetic behavior only.

Objectives

The most extensively studied graphene nanoribbons have two zigzag(z1) edges or two armchair(a11) edges. The former is antiferromagnetic but the latter is nonmagnetic. We want to show that theoretically we can make a graphene nanoribbon, no matter it has a zigzag or an armchair edge, ferromagnetic, or antiferromagnetic, or nonmagnetic by modifying the pattern of H-passivation at their two edges.

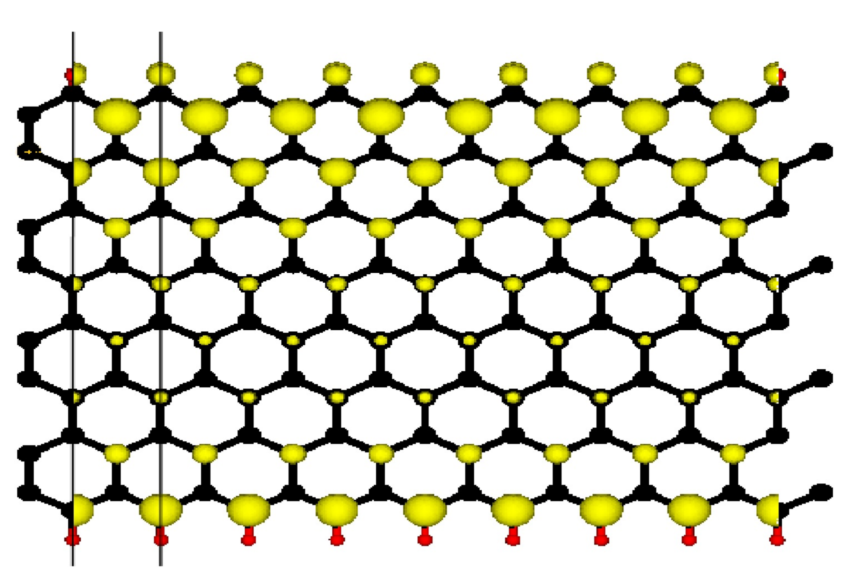
Methods

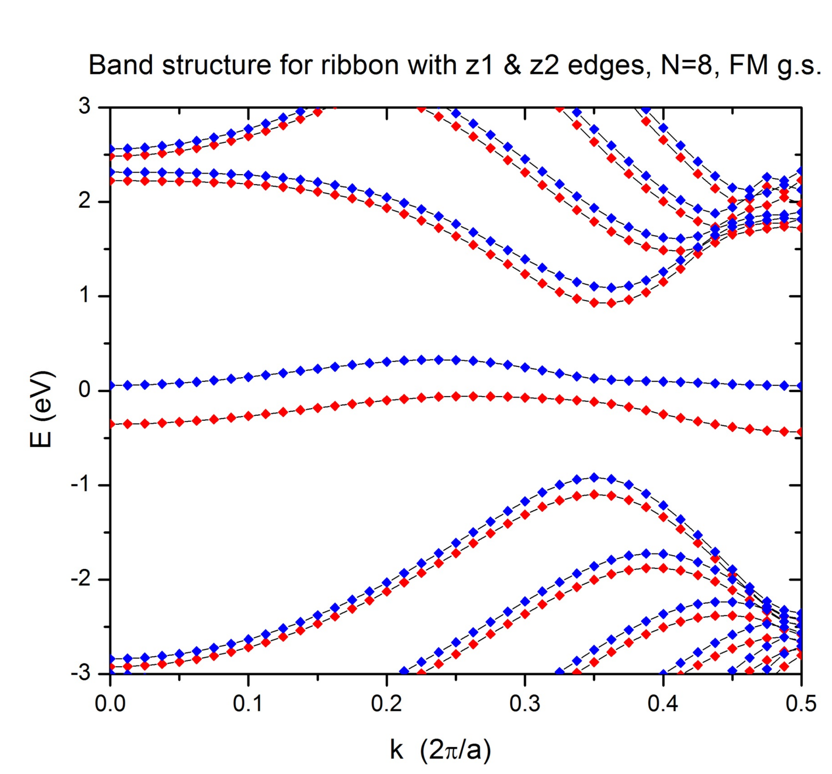
We use the local density approximation to Kohn-Sham density functional theory, executed in the VASP code. The structures were first optimized in a non-spin calculation. After the structures were optimized, a spin-dependent calculation was performed to obtained the energy spectrum and spin-density for both spin-up and spin-down electrons.

Results

1.**Graphene nanoribbon with a z1 edge & a z2 edge exhibit a ferromagnetic ground state**

g.s. spin density

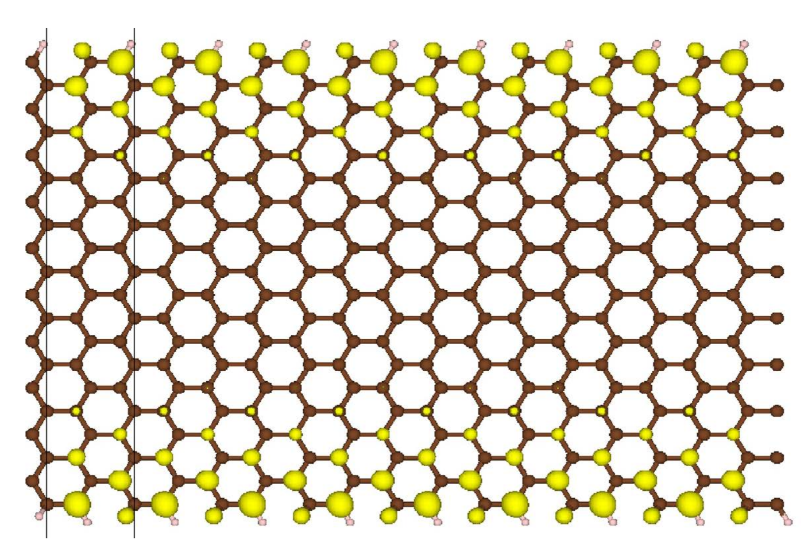


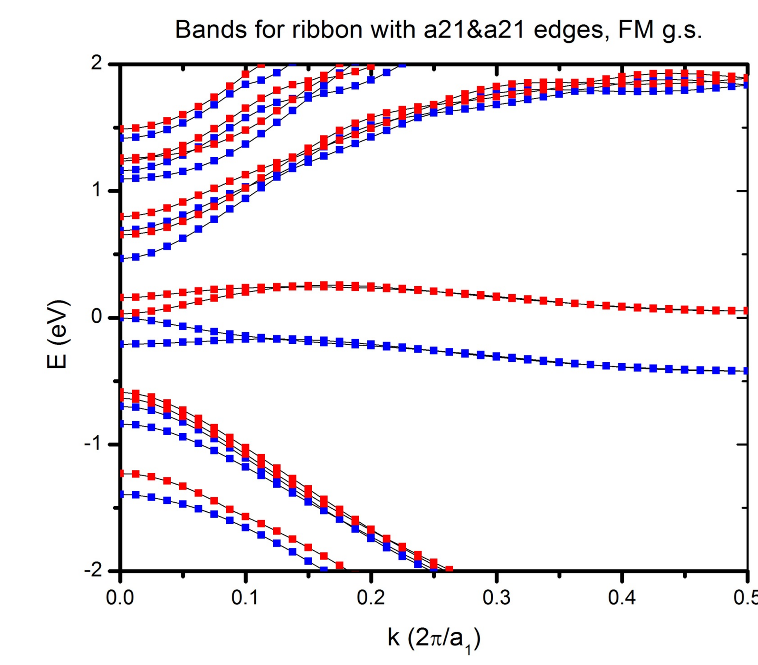


Results(continued)

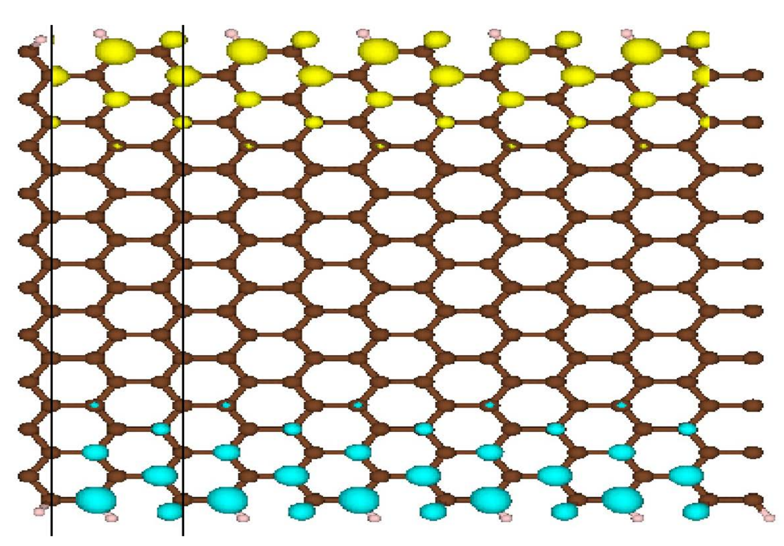
2.Graphene nanoribbon with two a21 edges exhibits a ferromagnetic g.s.

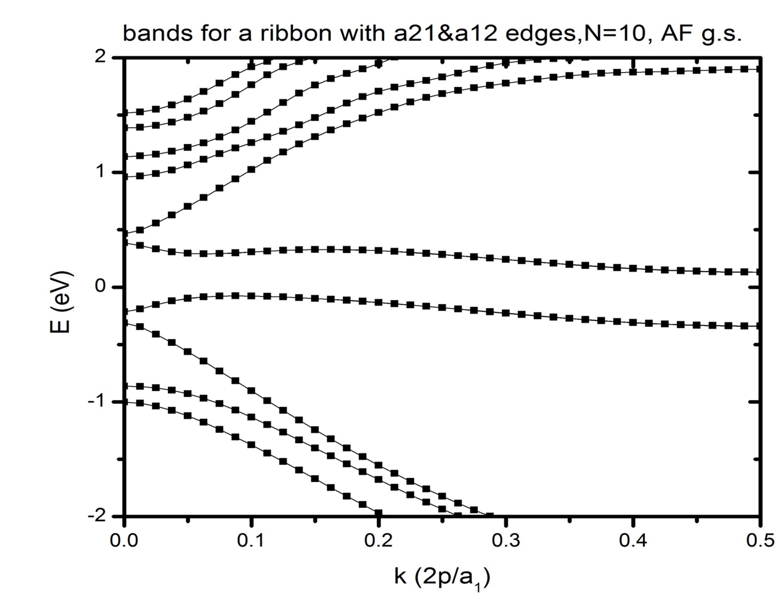
spin-density



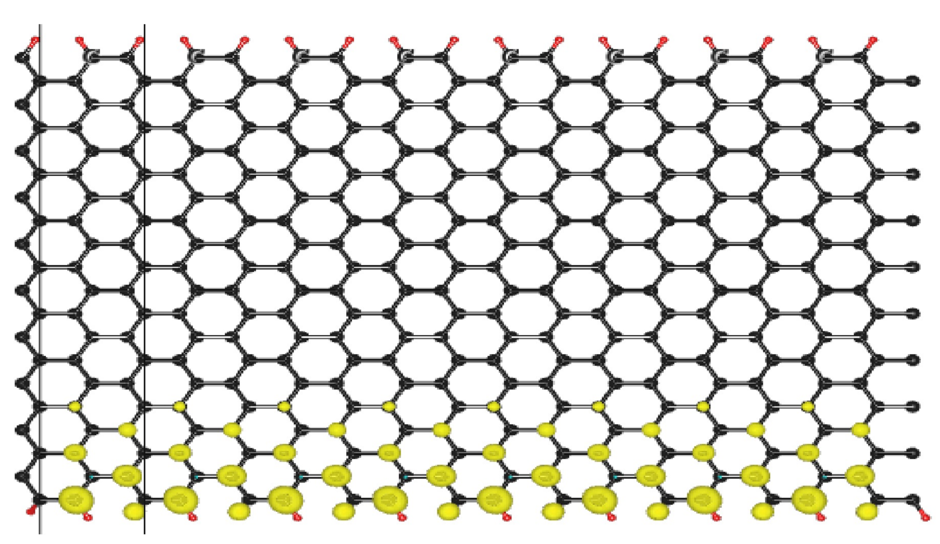


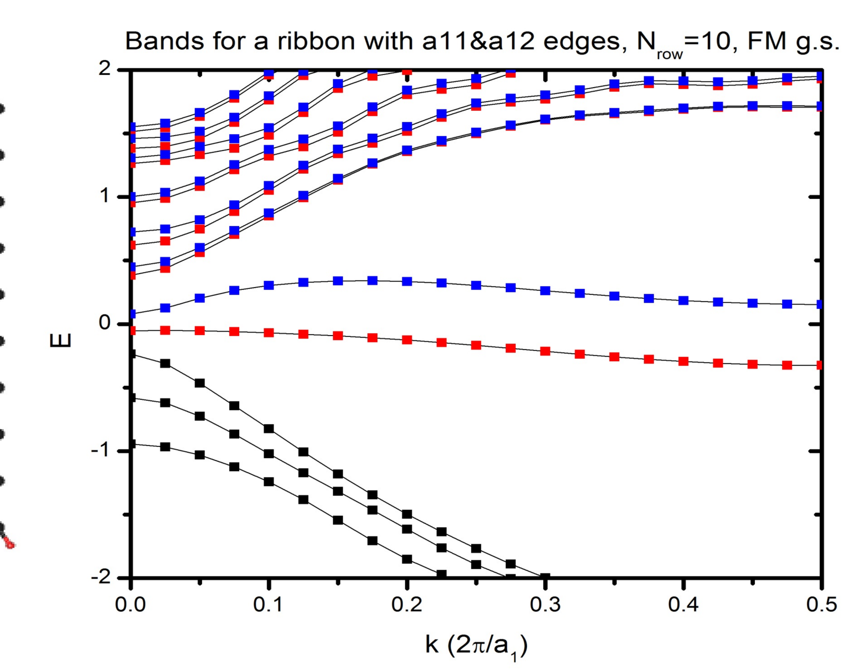
3. Graphene nanoribbon with an a21 & an a12 edges exhibits an anti-ferromagnetric g.s..





4. Graphene nanoribbon with an a11 and an a12 edges exhibits a FM g.s.





Conclusion

We can make graphene nanoribbons ferromagnetic, antiferromagnetic, or nonmagnetic by edge engineering.

References

[1]. W.Y. Ruan, Y.Y. Sun, S.B. Zhang, and M.Y. Chou, Origin of Magnetism in Graphene Derivatives(unpublished).

[2]. Y.Y.Sun, et. al., Graphene Nanoribbons and Band Gap Bifurcation of Dirac Fermions under Quantum Confinement, Phys.Rev. B (to be published).