# Novel Electronic States in Graphene Ribbons
## –Competing Spin and Charge Orders–

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### Introduction

New materials composed of carbon atoms, such as carbon nanotubes, are attracting much attention in both sides of fundamental science and their potential application to nanotechnology devices. In particular, nanographenes show various natures depending on their structures. For example, theoretical calculations [1] predict that localized magnetization appear along their zigzag-edges, not along their armchair-edges. In the present paper, we demonstrate novel electronic states in graphite ribbons which have unique physical characters originating from interplay of topologically different structures and Coulomb interactions. When a ribbon is twisted to make a Moebius strip, two kinds of electronic states appear: a *magnetic domain wall (MDW) state* [2] and a *helical magnetic(HM) state*. We also introduce a *ferroelectrically charge-separated (FECS) state with oppositely charges on both edges, resulting finite electric dipole moment pointing from one edge to the other*. This state is stabilized by the Coulomb interaction between the nearest neighbor sites. Our theoretical model is the extended Hubbard model with the on-site Coulomb repulsion $U$ and the nearest neighbor one $V$. We solved this model by developing a generalized scheme of the unrestricted Hartree-Fock (UHF) method which allows the mixing of up- and down-spin molecular-orbitals.

### Domain wall and helical magnetic states in a Moebius strip

We show spin density distributions of the MDW and HM states for Moebius strip in Fig.1(a) and (b),respectively for the case of $U=t$ and $V=0$ with the system size of 4x20 carbon sites ($t$ is the hopping integral between the nearest neighbor sites). Both states are characteristic in the Moebius geometry. In the MDW state, the domain walls interface two opposite ferrimagnetic orders of spins as shown in Fig.1(a). In the ferrimagnetic regions, spins are localized along the edges with larger magnitude at the two-fold coordinated sites than at three-fold coordinated sites. The HM state in Fig. 1(b) has a similar ferrimagnetic feature localized along the edge but the direction of spins rotates gradually and uniformly along the edge. It changes by $2\pi$ during the travel along both edges to return to the starting point. Therefore, it shows the helical ferrimagnetic order. In the case of much larger on-site interaction (for example, $U=10t$), the spin densities become comparable between at the two-fold and three-fold coordinated sites along the edges as well as inside the ribbon. This means that in both states the ferrimagnetic feature changes to the antiferromagnetic one with increasing *U*. We found that in the parameter region of $0<U<10t$, the HM states are enegetically more stable than the MDW states for the present system size.

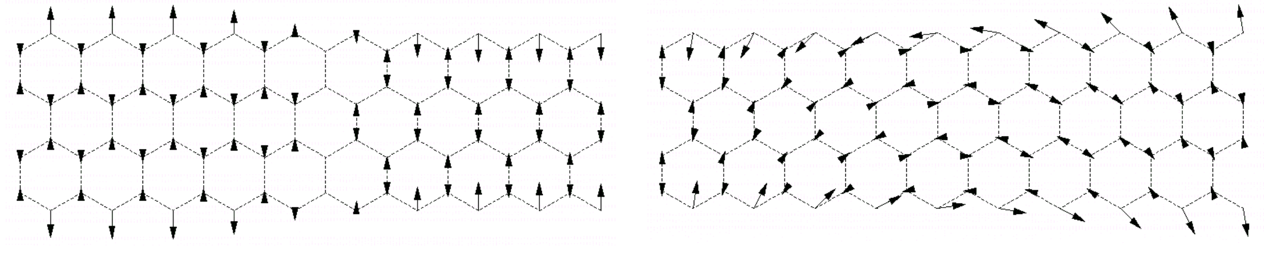
**Ferroelectrical charge-separated state**

We found out theoretically the novel *FECS* state with permanent electric dipole moment. Figure 2 shows the charge density distribution of this state in the case of $U=V=0.4t$ with the ring geometry. The electric charges are localized along the edges and their signs are opposite to each other. This indicates the existence of electric dipole moment pointing from one edge to the other. Net charge along each edge arises from much larger charge density at the tow-fold coordinated sites than at the three-fold coordinated ones. The magnitude of the electronic dipole moment per unit cell is 4.3 Debye, in the aforementioned parameters. We stress that this exotic dipole moment is spontaneously induced by the ring geometry and the nearest neighbor repulsion *V* in spite of the inversion symmetry of the system. The FECS state is energetically stabler than the localized magnetization (LM) state with no electric dipole moment when the effect of *V* overcomes that of *U*. Even in the parameter region where the LM state is the ground state, the external electric field stabilizes the FECS state. Further discussions and effects of *V* in the case of Moebius strip and graphene ribbons doped with electrons or holes will be presented in the conference.

**References**

[1] M. Fujita et. al, J. Phys. Soc. Jpn. **65** (1996) 1920.

[2] K. Wakabayashi and K. Harigaya, J. Phys. Soc. Jpn. **72** (2003) No. 5.



(a) (b)

Fig.1. Spin distributions of (a) the magnetic domain wall, and (b) helical magnetic states on a Moebius strip. The arrows represent spins on each carbon atom. The $S_y$ components are zero at all sites.

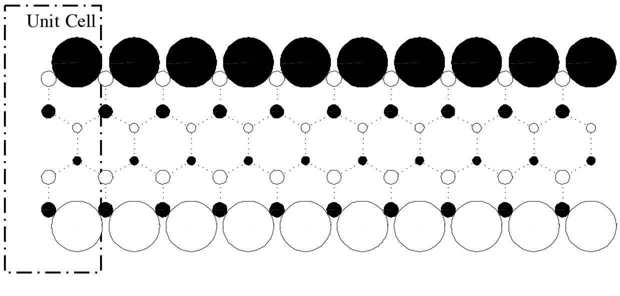


Fig.2. Charge density distribution of ferroelectrical charge-separated state on ring strip. Black and white circles represent positive and negative charge densities, respectively. The calculation was done for 4x40 carbons, and only the half is shown here.