Topological Phase in Graphene Nanoribbons

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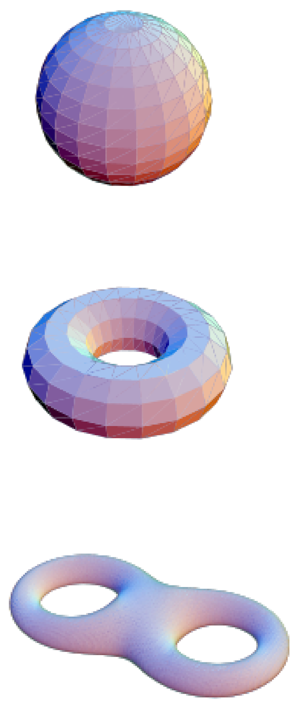
❖ Introduction

Topological Insulators are a class of materials that have robust conducting states at the boundary but are insulating in the bulk. The unconventional boundary states can be dissipationless or spin-momentum locked transport channel. Thus topological insulators have very promising applications in spintronics and novel electronics devices. The previous research of topological insulators focus on 2D or 3D systems, however, topological phase can also exist in one-dimensional system. Graphene nanoribbons, as a 1D carbon nanostructure, has been reported to host topological phase, which is manifested as localized end states or junction states. The topological phase in carbon nanostructures can be used to build quantum spin chain, spin qubit, or to realize Majorana fermions.

❖ Concept of Topology

Topological invariant of 3D geometry (real space):

$$\chi = \frac{1}{2\pi}\int_S \boldsymbol{G}\cdot d\boldsymbol{S} = \frac{1}{2\pi}\int_S \frac{1}{r^2}\cdot d\boldsymbol{S} = \begin{cases} 2 \\ 0 \\ -2 \end{cases}$$

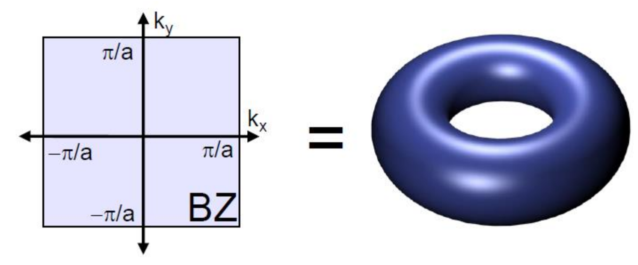


χ **:** Topological invariant

$\boldsymbol{G}$ **:** Gaussian curvature

$\boldsymbol{S}$ **:** Geometric surface in real space

Topological invariant of 2D BZ (reciprocal space):



2D Brillouin zone (BZ) is a torus

$$n = \frac{1}{2\pi}\sum_n \int_{BZ} \boldsymbol{\Omega}^n_{k_x,k_y}\cdot d\boldsymbol{k}$$

n **:** Topological invariant

$\boldsymbol{\Omega}$ **:** Berry curvature

BZ**:** Brillouin zone (torus in reciprocal space)

❖ Theory of Topological Phase in 1D Structures

The topological phase in 1D carbon nanostructure is characterized by $\mathbb{Z}_2$ invariant.
Definition of $\mathbb{Z}_2$ invariant is given by:

$$\gamma_n = \int_{BZ}\langle u_{n,k}|\partial_k|u_{n,k}\rangle = \gamma_n^{\text{intra}} + \gamma_n^{\text{inter}} \qquad (-1)^{\mathbb{Z}_2} = \exp\left(i\sum_n^{\text{occ}}\gamma_n^{\text{inter}}\right)$$

where γ_n^{inter} is intercellular Zak phase, "occ" means occupied bands.
The Zak phase is also related to Wannier centre through the following formula:

$$\bar{x} = \sum_n \bar{x}_n = \frac{a}{2\pi}\sum_n \gamma_n^{\text{inter}}$$

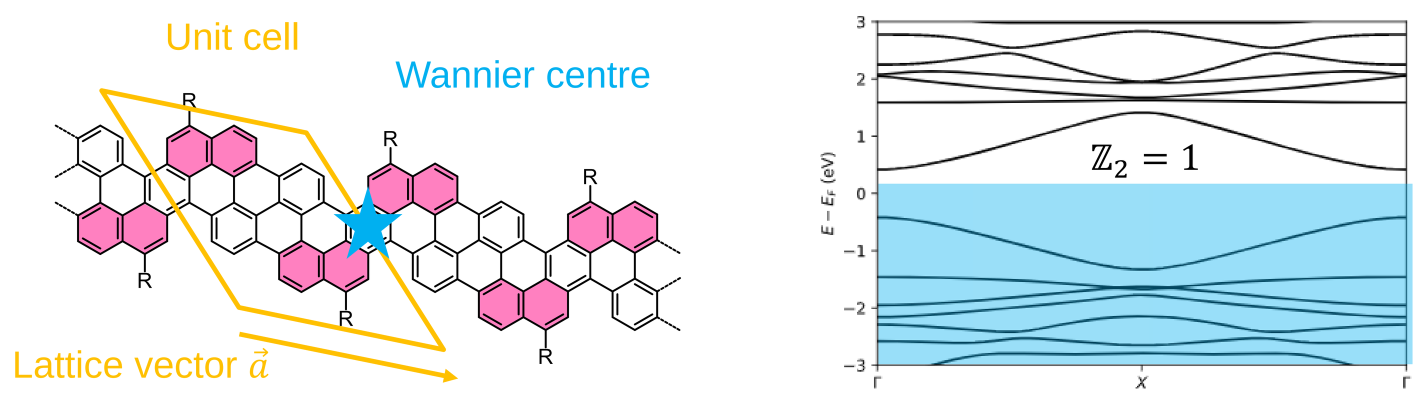
Therefore, we can investigate the topological phase of a structure by calculating the $\mathbb{Z}_2$ invariant or Wannier centre.

Methodology:

- Calculating $\mathbb{Z}_2$ invariant
- Calculate Wannier centre
- Calculate Local Density of States (LDOS)

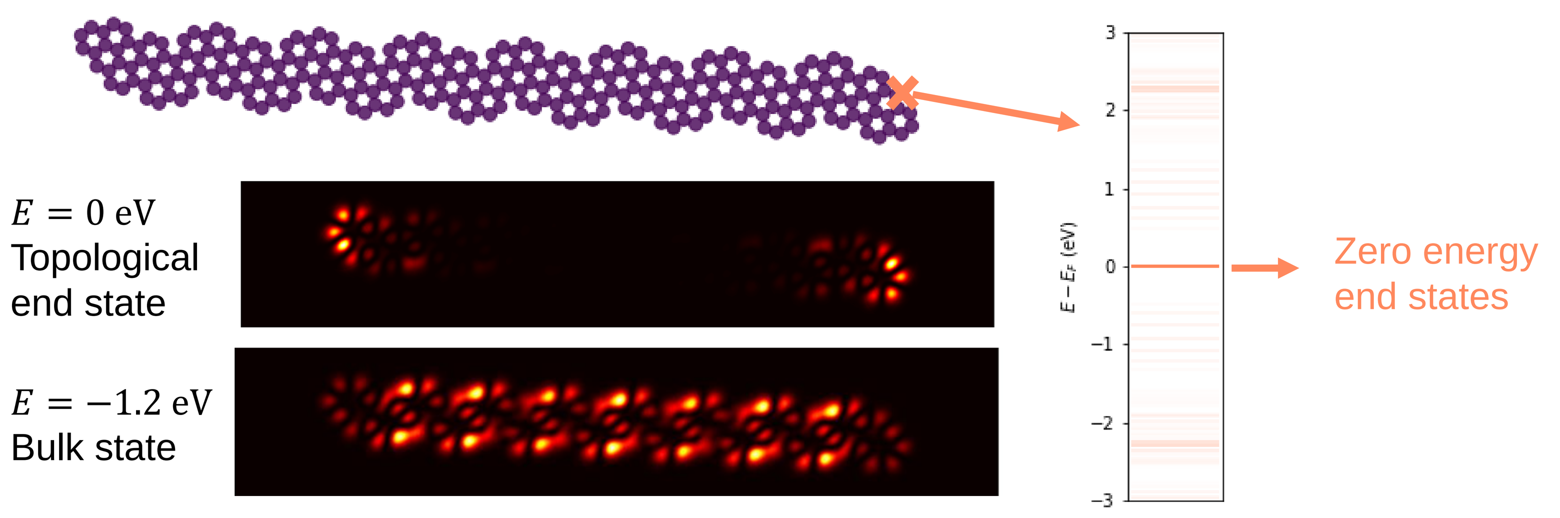
	Trivial	Non-trivial
$\mathbb{Z}_2$	0	1
Zak phase	0	π
Wannier centre	0 (unit cell centre)	$a/2$ (unit cell boundary)
LDOS	No end states	In-gap end states

❖ Topological Non-trivial and Trivial Graphene Nanoribbons



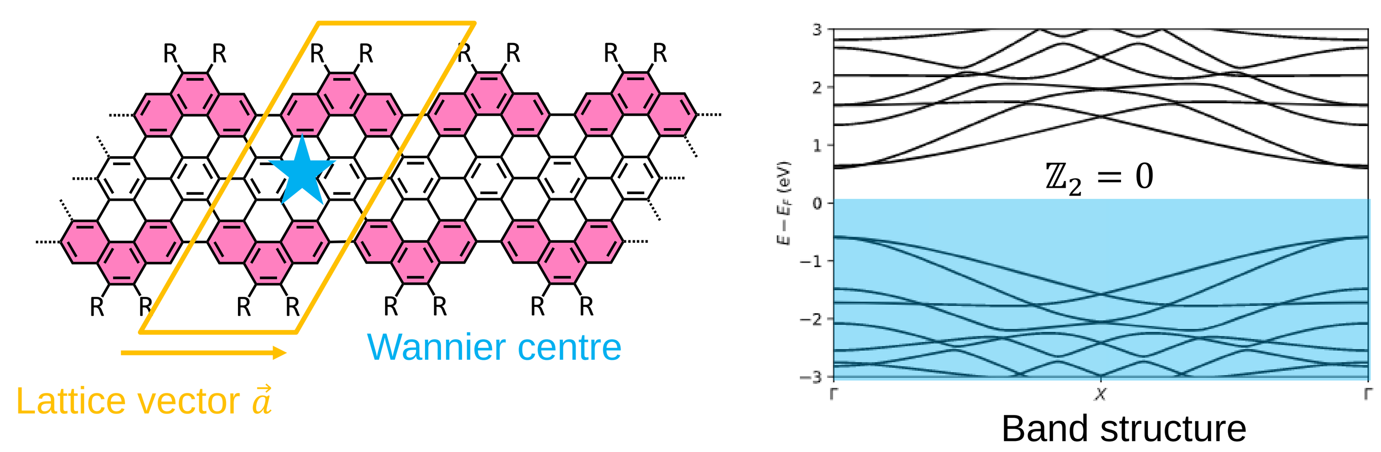
Finite GNR with 8 unit-cells

Band structure



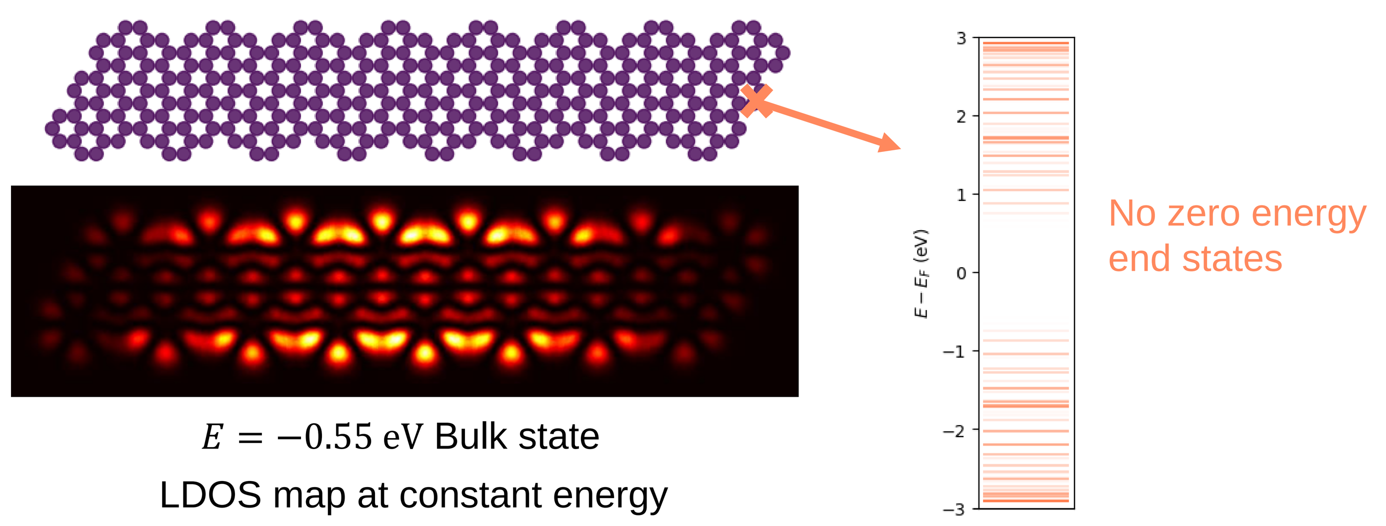
LDOS map at constant energy

LDOS



Finite GNR with 8 unit cells

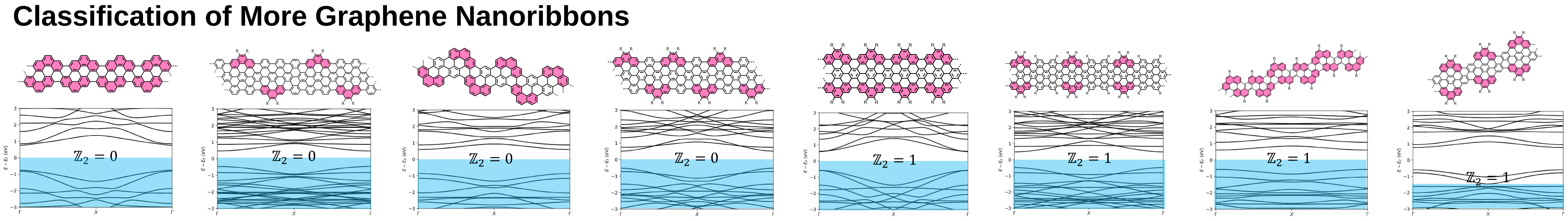
Band structure



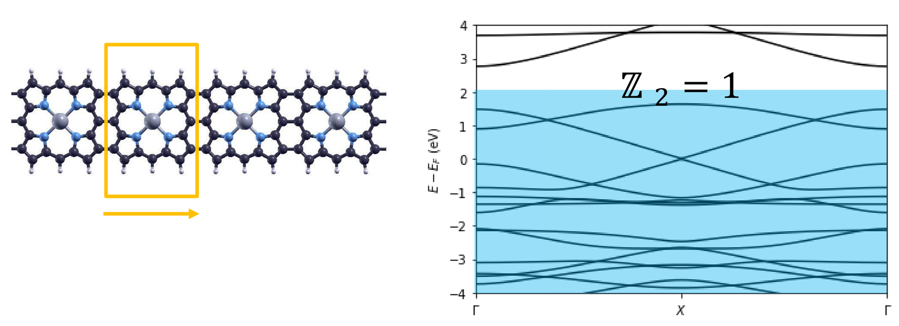
$E = -0.55$ eV Bulk state

LDOS map at constant energy

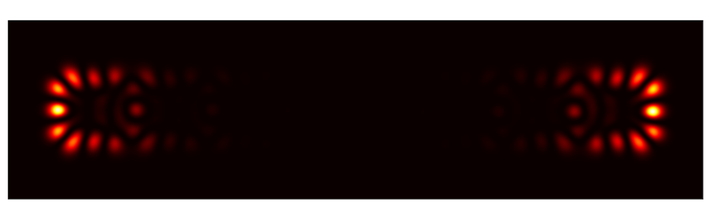
❖ Classification of More Graphene Nanoribbons



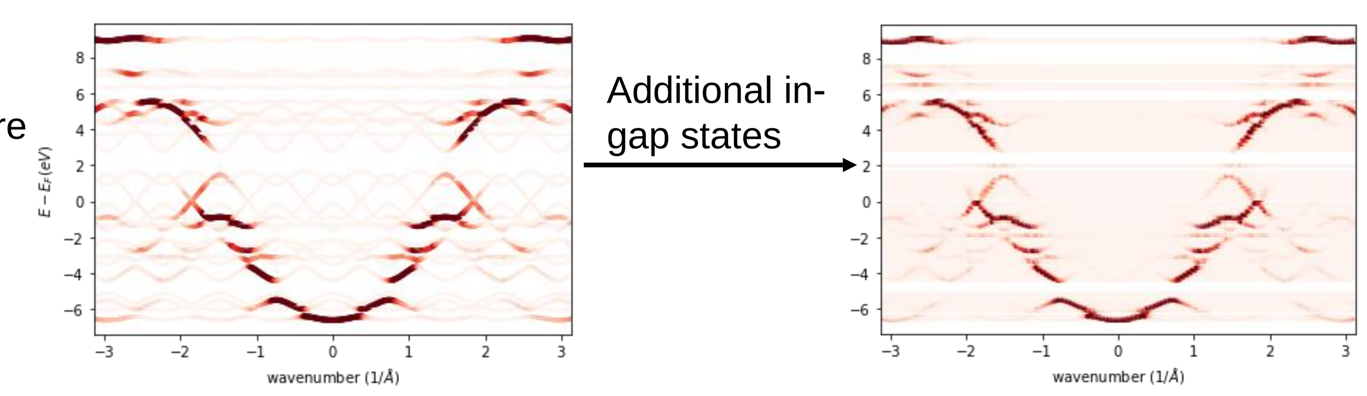
❖ Topological Phase in Porphyrin Structures



Topological end states of finite porphyrin ribbon at $E = 2.0$ eV :



Unfolded band structure with periodic boundary condition



Unfolded band structure of 8 unit-cell finite chain

❖ Conclusions

- Topological phase exists universally in carbon nanostructures like graphene nanoribbons and porphyrin nanoribbons. The latter is not reported before.
- The classification of topological phase provides guidance to chemical synthesis, so that we can focus on the synthesis and following characterization of topologically interesting molecules.
- Topological phase in carbon nanostructures is a thriving research field that will find its application in spintronics, nano-electronics, and quantum information technology.

1. Rizzo, Daniel J., et al. "Topological band engineering of graphene nanoribbons." Nature 560.7717 (2018): 204-208.
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