Progress in graphene nanoribbon project: 
Topological band engineering & metallic GNRs

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Some important issues on GNRs for nanoelectronics

- GNRs with appropriate band gaps for transistors and other applications
- GNRs as metallic wires
- Very narrow-band metallic GNRs to beat the 60 meV/decade switching limit
Outline of Talk

• Topological quantum band engineering
  - Topological invariants and junction states in GNRs
  - Engineering band gap with topology

• Design and synthesis of metallic GNRs
  - Dopants and structural changes
  - Electron topology
Bottom-up synthesis of GNRs with precursor molecules

- Perfect arm-chair or zigzag GNRs of widths (~1-3 nm) and lengths (~50-100 nm) synthesized on surfaces or in solutions


- Heat 13-AGNR

Bottom-up synthesis of GNRs with precursor molecules

- Heat 7-13-AGNR junctions

Background: Graphene Nanoribbons (GNRs) - Bandgap vs. Width

Armchair GNR

• Large band gap for most GNRs due to quantum confinement & large self-energy effect from strong many-electron interactions

• Band gaps decrease with width, but bottom-up synthesized GNRs have very narrow width

• Engineer small bandgap ribbons from large bandgap ribbons by using a novel topological concept

Topological phases in graphene nanoribbons

- Electron states confined in BZ, a compact geometric manifold. Distinct topology!

- Non-trivial topology of Bloch bands $\Rightarrow$ protected boundary states, integer quantum Hall effect, new phases of matter, ... (Nobel prize 2016 – Thouless, Haldane, Kosterlitz)

- Symmetry protected topological (SPT) phases in 1D $\Leftrightarrow$ quantized Berry phase (intercell) $\gamma$ across the BZ of all the occupied bands, which may be specified by an invariant: $Z_2 = 0$ or 1

$$(-1)^{Z_2} = e^{i\sum_n \gamma_n}$$

$Z_2 = 0$ (trivial) (Regular strip)

$Z_2 = 1$ (non trivial) (Mobius strip)

Cao, Zhao and Louie, *PRL* 119, 076401 (2017)
Topological phases in graphene nanoribbons

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• Symmetry protected topological (SPT) phases in 1D ⇔ quantized Berry phase (intercell) $\gamma$ across the BZ of all the occupied bands, which may be specified by an invariant: $Z_2 = 0$ or 1

\[ (-1)^{Z_2} = e^{i \Sigma_n \gamma_n} \]

• Discovered all GNRs (with spatial symmetry) are large gap insulators that host SPT phases

• Bulk-boundary correspondence ⇒ boundary states between topological distinct segments

• $Z_2$ can change with different terminating unit cell (it changes the Berry’s phases)

Cao, Zhao and Louie, *PRL* 119, 076401 (2017)
GNR Heterostructure: Topological vs. non-topological

9-AGNR/7-AGNR heterostructure

Topologically equivalent
No interface state!

Cao, Zhao and Louie, *PRL* 119, 076401 (2017)
Topological Quantum Engineering: Creating topological bands in 7-9 AGNR superlattices

- Eg (7-AGNR) > Eg (9-AGNR) \(\Rightarrow\) Longer decay length in 9AGNR
- Bigger coupling through N=9 than N=7: \(|t_1| > |t_2|\)
- *Topological junction states* form 2 bands within the bulk band gap whose properties may be tuned with the length of the segments.

Symmetric vs. Asymmetric Superlattices

- Band gap difference between the two configurations arise from topological effects.
- Gap values correspond to system on metal substrate.
Bond-resolved STM Image of 7-9 GNR Superlattice

BRSTM imaging parameters: \( \frac{dI}{dV} \) image
\( V_{DC} = 20 \text{ mV}, V_{AC} = 12 \text{ mV}, I = 80 \text{ pA} \) (feedback on)

Spectroscopy vs. Theory for Topological 7-9 GNR Superlattices

- Can change the bandgap and bandwidth by changing the segment lengths!
- Expect a magnetic ground state if the on-site Coulomb $U > Eg \sim 2t_1$.
- Stable spin centers (magnetism) develop with bigger $U$ or smaller $t_1$.

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Nitrogen doped 7AGNRs as metallic leads

- Nitrogen doped GNRs can be good metals.
- 7AGNR/7AGNR-4N junction *likely* has an ohmic contact.

Lee, Cao, Zhao and Louie (2018)
Cove-edged GNRs as metallic leads

- Gapless for width $N = \text{even}$, asymmetric staggering case
- Should be a good metal

Lee, Zhao, Cao and Louie, accepted by *Nano letters*
Boron-dimer periodic-doped GNRs as narrow band metallic leads

- Nearly dispersionless boron-dimer-induced bands because of symmetries
- When doped very narrow metallic bands (both small $t$ and $U$)

Cao, Zhao and Louie, *PRL* **119**, 076401 (2017); ibid, to be published.
Engineering Metallic GNRs from Topological Superlattices

\[ E_g = 2 |t_1 - t_2| \]

Semiconductor Band Structure for: \( t_1 \neq t_2 \); \( E_g > 0 \)

Metallic Band Structure for: \( t_1 = t_2 \); \( E_g = 0 \)

(Fischer, Crommie and Louie groups)
Possible Ultra-Small Bandgap Graphene Nanoribbons: 4,4-9-AGNRs

F. Fischer group
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The Louie Group (2018)