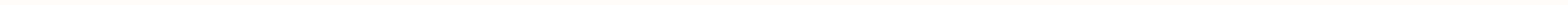


Computational Physics Final Presentation

Band Structure of Graphene Nano-Ribbon Using Tight Binding Model

NYCU MSE 黃詠淳 Yung-Chun, Huang



1. Band Structure of Graphene

Analytical

Numerical

2. Band Structure of Graphene Nanoribbon

What are Graphene Nanoribbons?

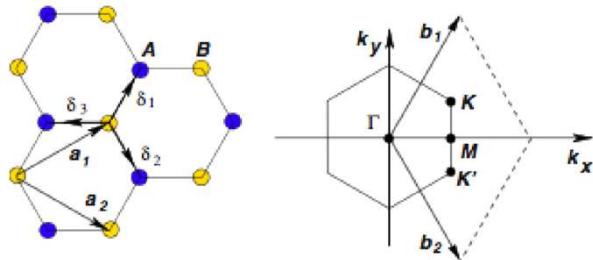
Constructing the Tight-Binding Model

3. Discussions

4. Demo

Band Structure of Graphene.

Band Structure of Graphene



$$a_1 = \frac{a}{2}(\sqrt{3}, 1), a_2 = \frac{a}{2}(\sqrt{3}, -1)$$

$$\langle A|H|B\rangle = \langle A|T + \sum_n V_n^A + \sum_m V_m^B |B\rangle \quad (47)$$

$$= \frac{1}{N} \sum_{i'} \sum_i e^{i\vec{k} \cdot (\vec{R}_i^B - \vec{R}_{i'}^A)} \langle \varphi_{i'}^A | T + \sum_n V_n^A + \sum_m V_m^B | \varphi_i^B \rangle \quad (48)$$

$$\approx \frac{1}{N} \sum_{i'} \sum_i e^{i\vec{k} \cdot (\vec{R}_i^B - \vec{R}_{i'}^A)} \langle \varphi_{i'}^A | V_{i'}^A + V_i^B | \varphi_i^B \rangle \quad (49)$$

$$= \sum_i e^{i\vec{k} \cdot (\vec{R}_i^B - \vec{R}_0^A)} \langle \varphi_0^A | V_0^A + V_i^B | \varphi_i^B \rangle \quad (50)$$

$$\approx \sum_{i=1}^{N_{NN}} e^{i\vec{k} \cdot \vec{d}_i^{AB}} t_i^{AB}, \quad (51)$$

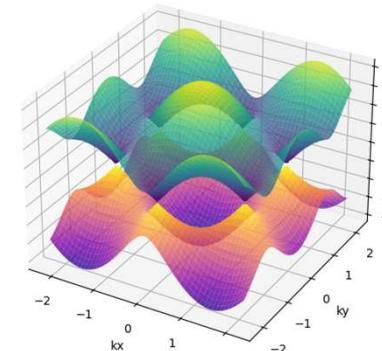
Hamiltonian

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i)$$

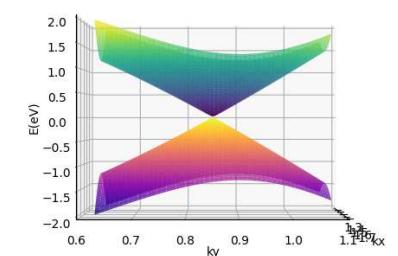
Analytical solution:

$$E(k) = \pm t \sqrt{1 + 4\cos^2\left(\frac{k_x a}{2}\right) + 4\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{\sqrt{3}k_y a}{2}\right)}$$

Energy Band of Graphene



Dirac Cone of Graphene

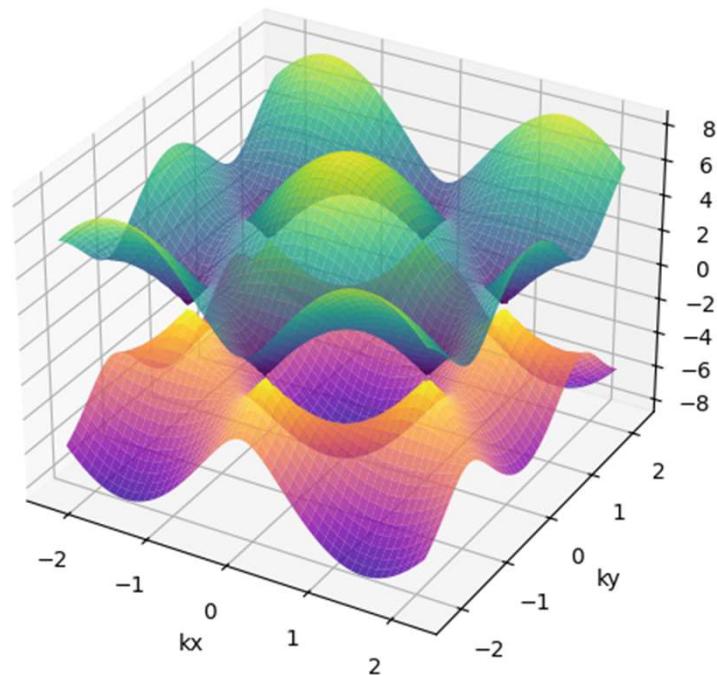


Parameters: $a = 1.24 \text{ \AA}$, $t = 2.8 \text{ eV}$

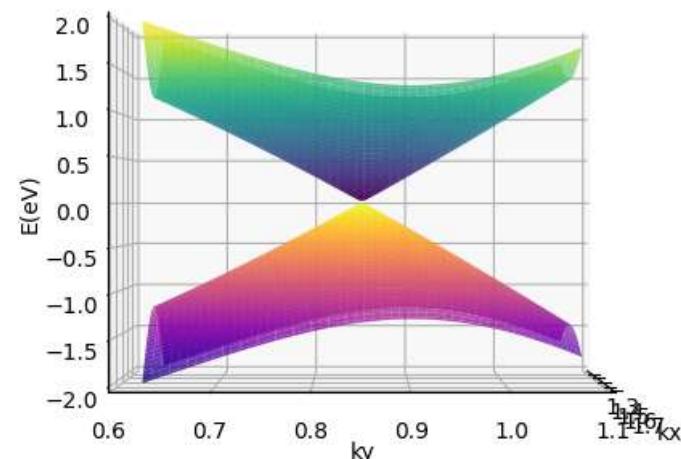
Plotting Analytical Solution

Parameters: $a = 1.24 \text{ \AA}$, $t = 2.8 \text{ eV}$

Energy Band of Graphene

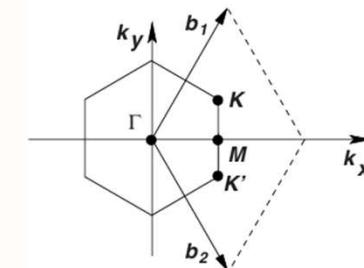
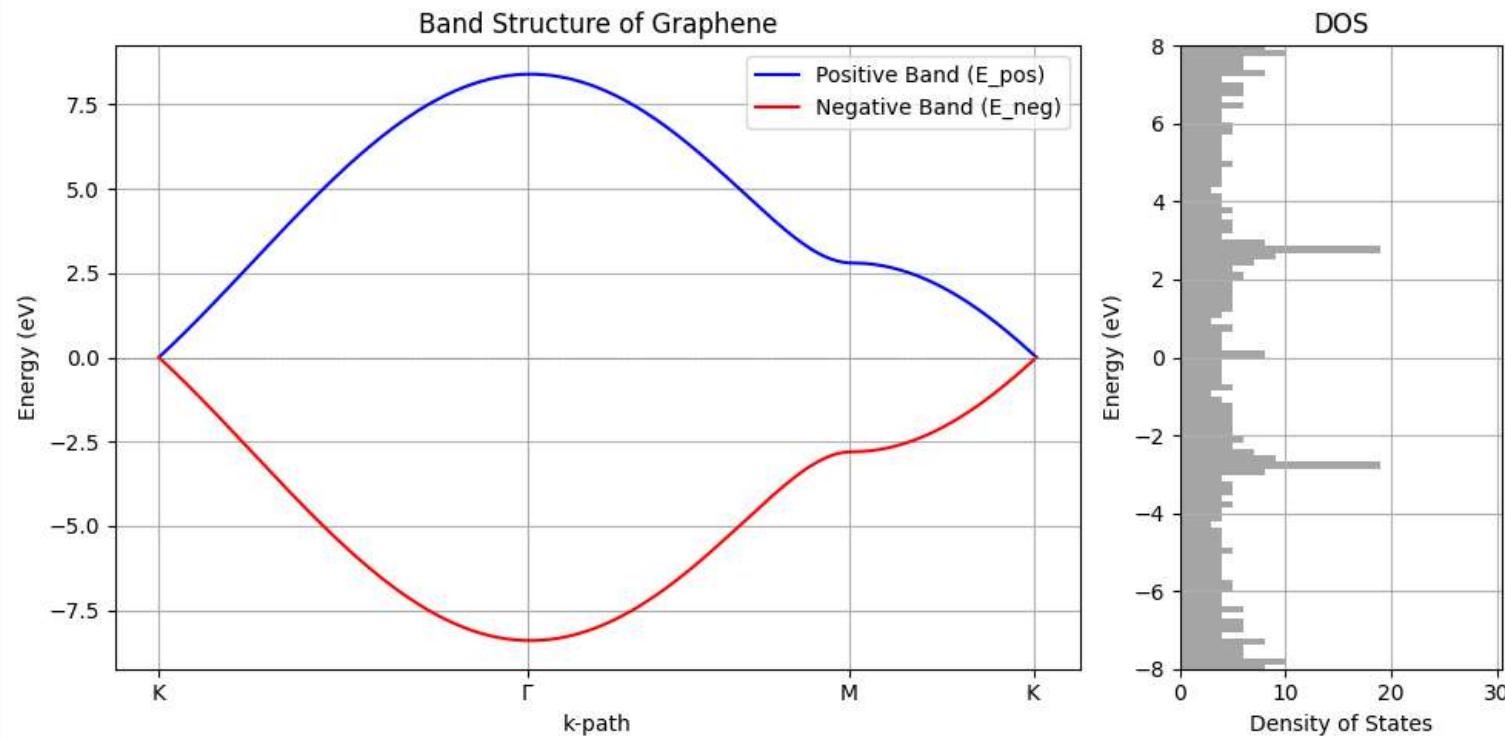


Dirac Cone of Graphene



Plotting Analytical Solution

Parameters: $a = 1.24 \text{ \AA}$, $t = 2.8 \text{ eV}$



Numerical Solution

Define Hamiltonian and solve for eigen values

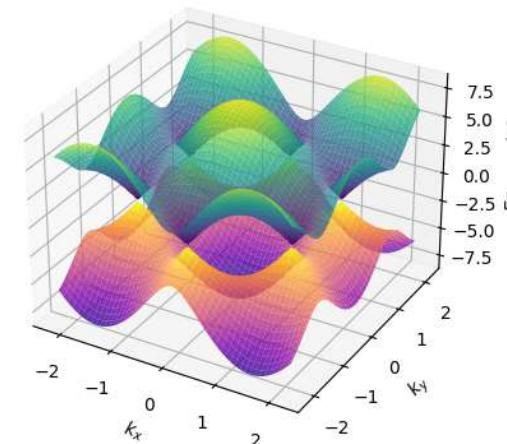
- The Hamiltonian matrix is constructed as:

$$H = -t(h_x\sigma_x - h_y\sigma_y)$$

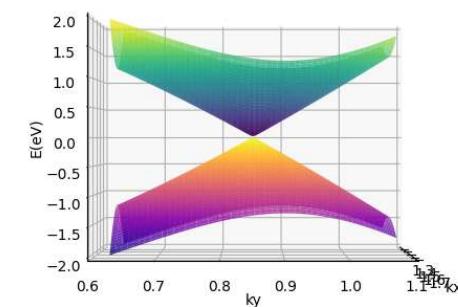
- h_x : Controls the coupling between sublattices through σ_x .
- h_y : Includes phase-dependent hopping through σ_y .
- $-t$: Scales the entire Hamiltonian by the hopping energy.

```
# Define the Hamiltonian matrix for graphene.
def Hamiltonian_Graphene(kx, ky):
    a = 1.42 # nearest neighbor distance
    t = 2.8 # Hopping parameter
    d1 = (a / 2) * np.array([1, np.sqrt(3)])
    d2 = (a / 2) * np.array([1, -np.sqrt(3)])
    d3 = -a * np.array([1, 0])
    sx = np.array([[0, 1], [1, 0]])
    sy = np.array([[0, -1j], [1j, 0]])
    hx = np.cos(np.dot([kx, ky], d1)) + np.cos(np.dot([kx, ky], d2)) + np.cos(np.dot([kx, ky], d3))
    hy = np.sin(np.dot([kx, ky], d1)) + np.sin(np.dot([kx, ky], d2)) + np.sin(np.dot([kx, ky], d3))
    H = -t * (hx * sx - hy * sy)
    return H
```

Graphene Band Structure

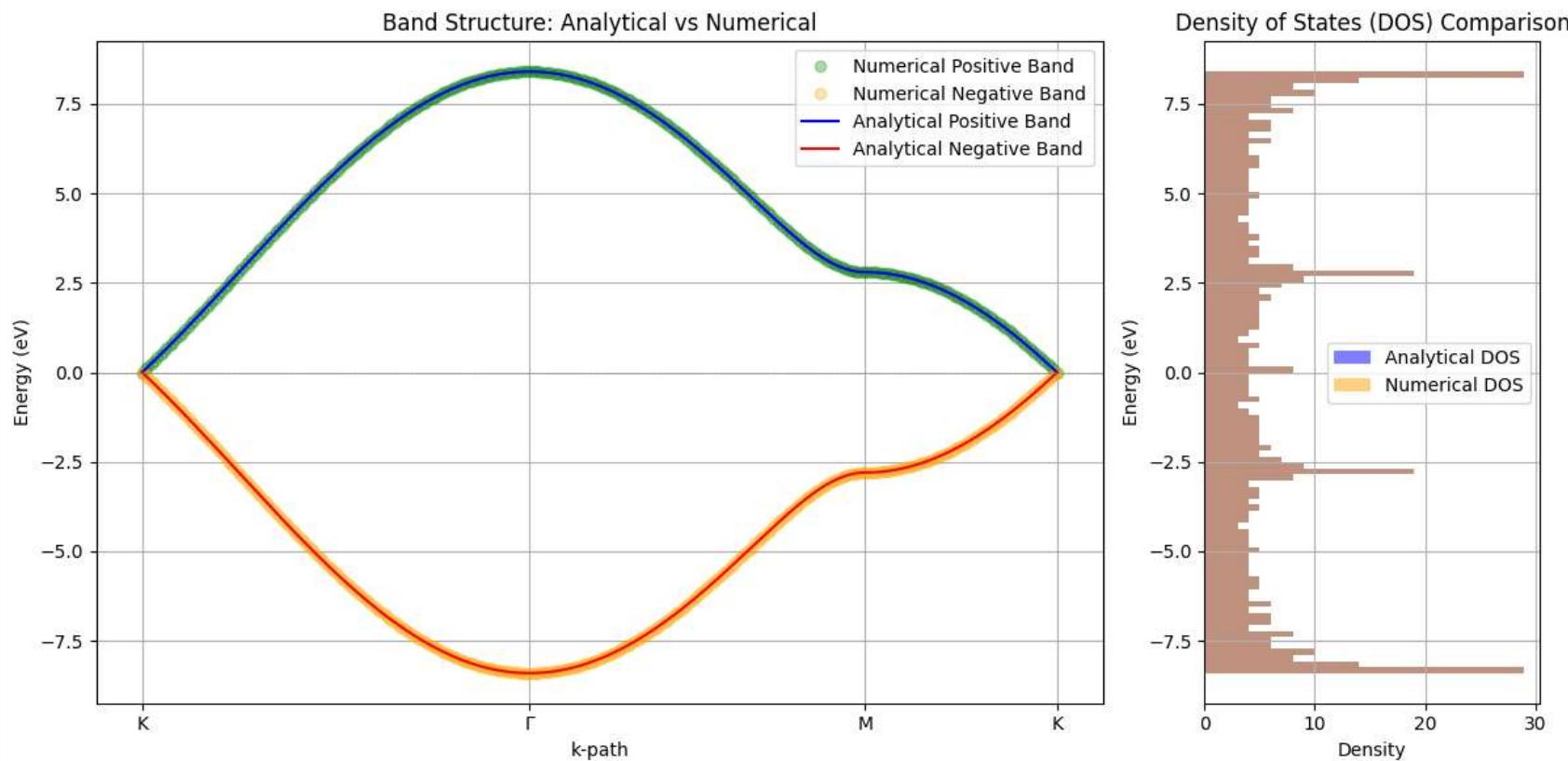


Dirac Cone of Graphene



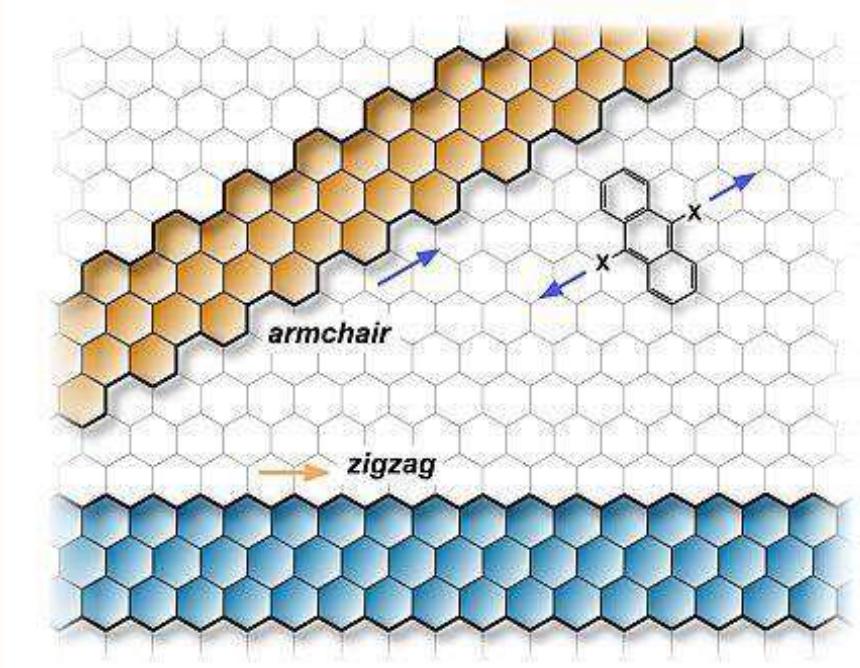
Analytical vs Numerical

Params: $a = 1.24 \text{ \AA}$, $t = 2.8 \text{ eV}$



Graphene Nanoribbon (GNR).

Graphene Nanoribbon (GNR)



(ref: [Nanoribbons: One-Dimensional Nanostructures with Unique Properties and Applications](#))

Importance of Studying GNRs

Promising for nanoelectronics, spintronics, and optoelectronics

Types of GNRs:

1. Armchair GNR (AGNR):

Smooth edges resembling an armchair pattern
Tunable bandgap (semiconducting or metallic-like)..

2. Zigzag GNR (ZGNR): Sharp zigzag-shaped edges.

Constructing the Tight-Binding Model

PRL 97, 216803 (2006)

PHYSICAL REVIEW LETTERS

week ending
24 NOVEMBER 2006

Energy Gaps in Graphene Nanoribbons

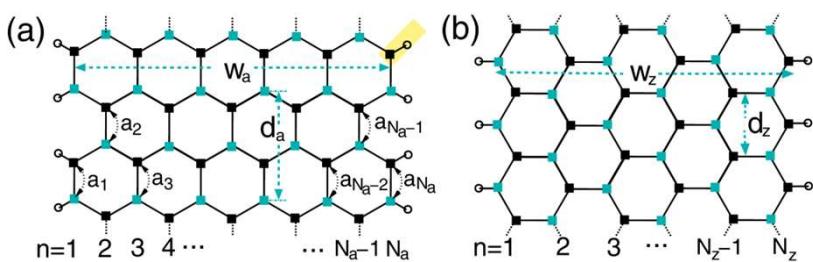
Young-Woo Son,^{1,2} Marvin L. Cohen,^{1,2} and Steven G. Louie^{1,2,*}¹Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA²Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

(Received 29 June 2006; published 22 November 2006)

Based on a first-principles approach, we present scaling rules for the band gaps of graphene nanoribbons (GNRs) as a function of their widths. The GNRs considered have either armchair or zigzag shaped edges on both sides with hydrogen passivation. Both varieties of ribbons are shown to have band gaps. This differs from the results of simple tight-binding calculations or solutions of the Dirac's equation based on them. Our *ab initio* calculations show that the origin of energy gaps for GNRs with armchair shaped edges arises from both quantum confinement and the crucial effect of the edges. For GNRs with zigzag shaped edges, gaps appear because of a staggered sublattice potential on the hexagonal lattice due to edge magnetization. The rich gap structure for ribbons with armchair shaped edges is further obtained analytically including edge effects. These results reproduce our *ab initio* calculation results very well.

DOI: 10.1103/PhysRevLett.97.216803

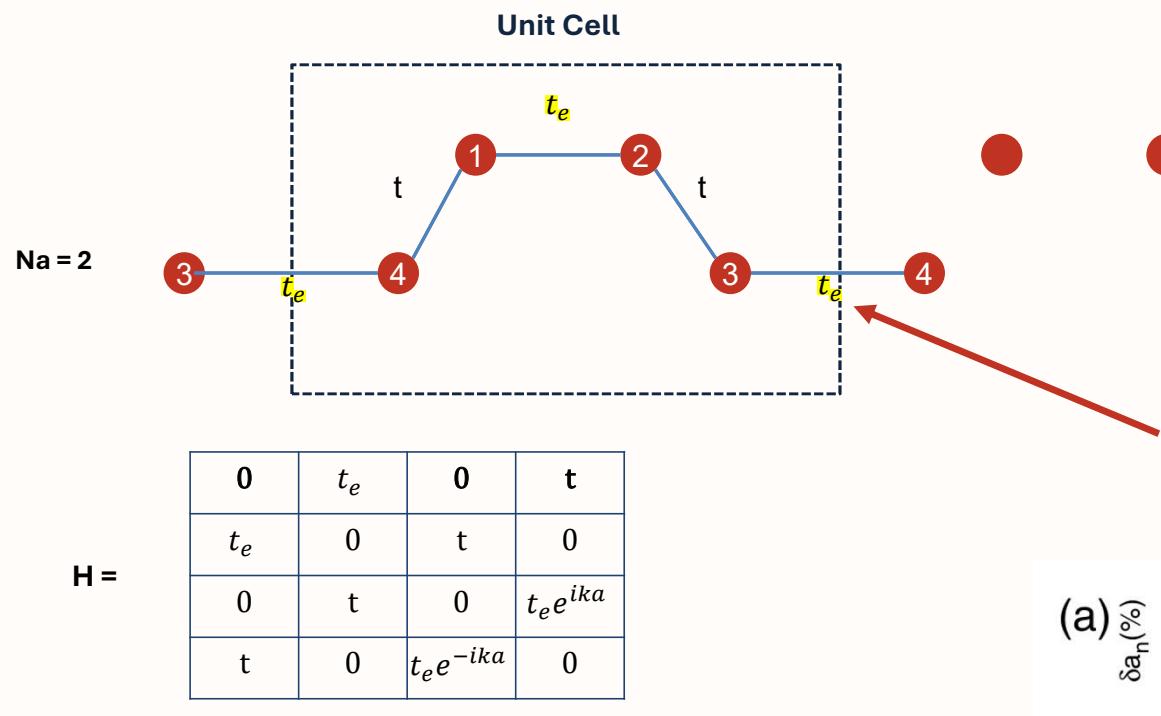
PACS numbers: 73.22.-f, 72.80.Rj, 75.70.Ak



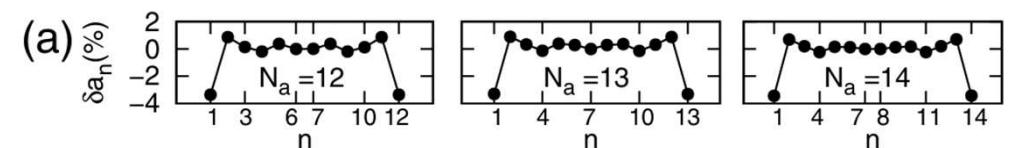
1. Hamiltonian Construction:
Basis: p_z orbitals of carbon atoms.
Hopping Parameter (t): t=2.7 eV

2. Defining Na:
Na: Number of dimer lines for AGNR
Bandgap is a function of Na.

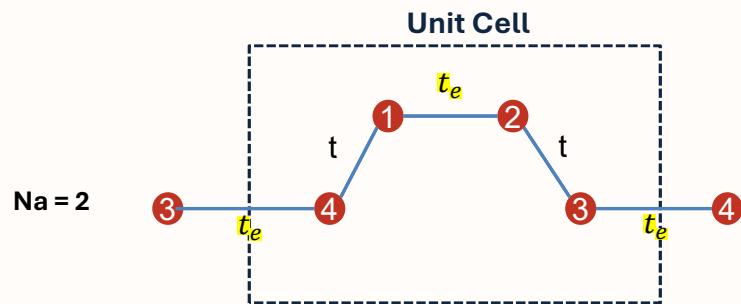
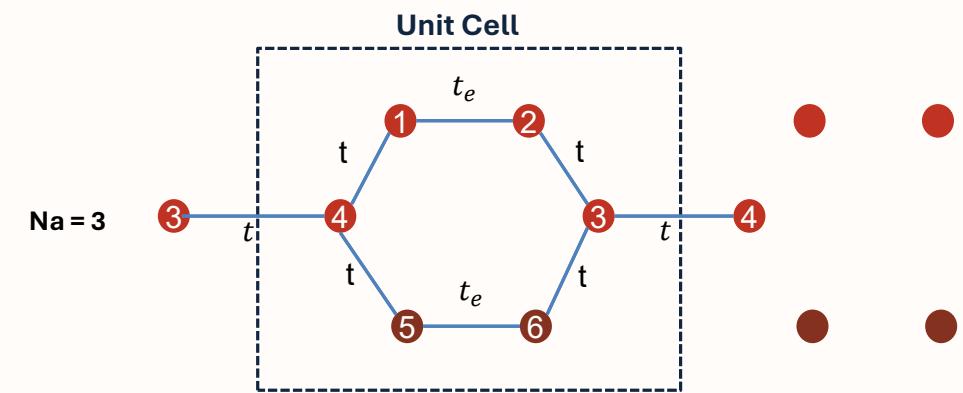
Constructing the Tight-Binding Model



“A 3.5% decrease in interatomic distance would induce a 12% increase in the hopping integral between orbitals.”



Constructing the Tight-Binding Model

 $N_a = 2$  $N_a = 3$ $H =$

0	t_e	0	t
t_e	0	t	0
0	t	0	$t_e e^{ika}$
t	0	$t_e e^{-ika}$	0

 $H =$

0	t_e	0	t	0	0
t_e	0	t	0	0	0
0	t	0	$t_e e^{ika}$	0	t
t	0	$t e^{-ika}$	0	t	0
0	0	0	t	0	t_e
0	0	t	0	t_e	0

And so
forth ...

See the
pattern?

Band Structure

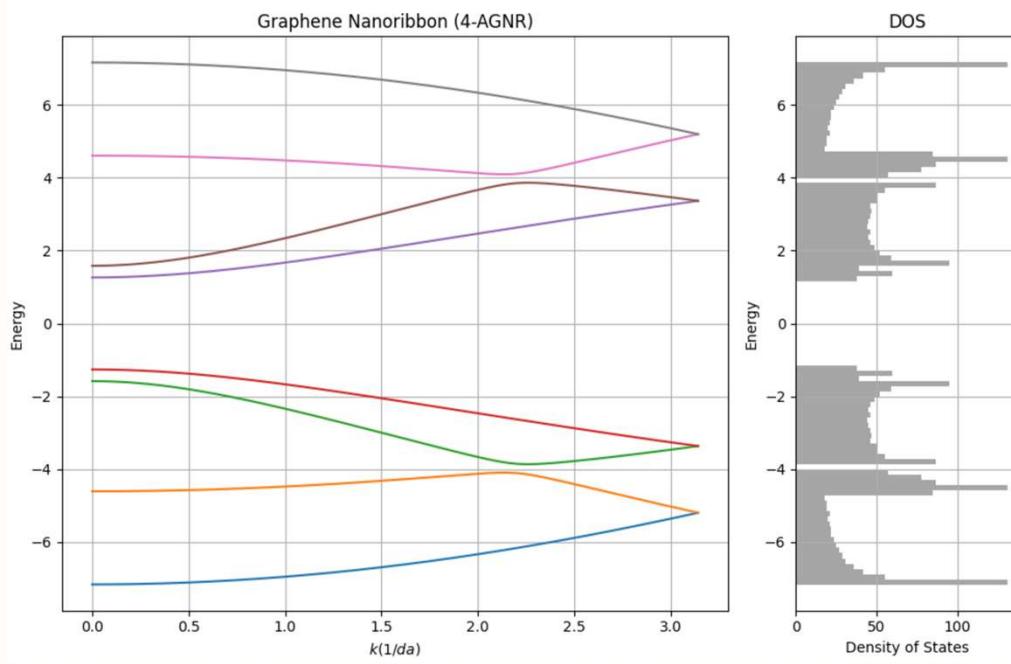
Mine vs Literature

$N = 4$

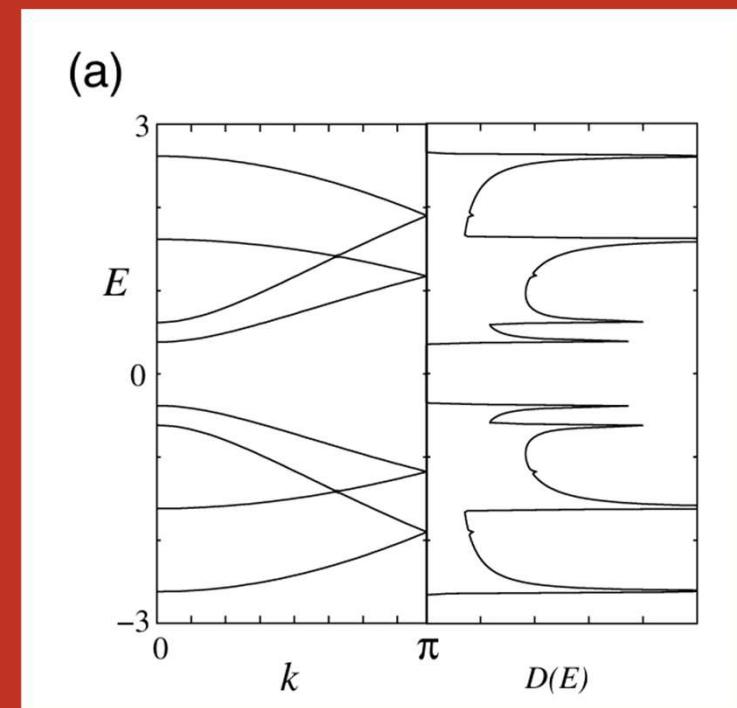
$a = 1.42 \text{ \AA}$

$t = 2.7 \text{ eV}$

My Calculation



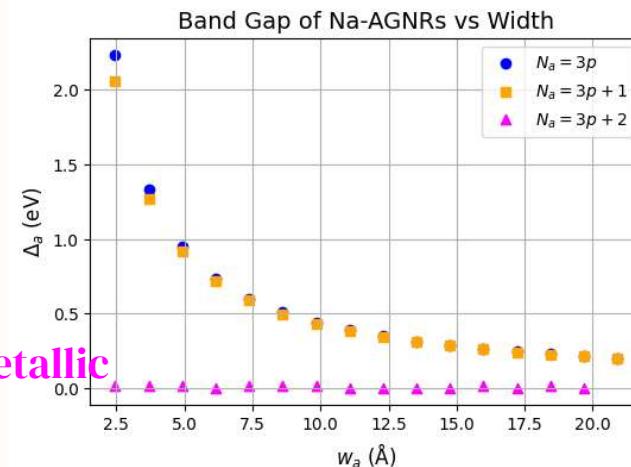
Wakabayashi, K., Sasaki, K. ichi, Nakanishi, T., & Enoki, T. (2010). Electronic states of graphene nanoribbons and analytical solutions.



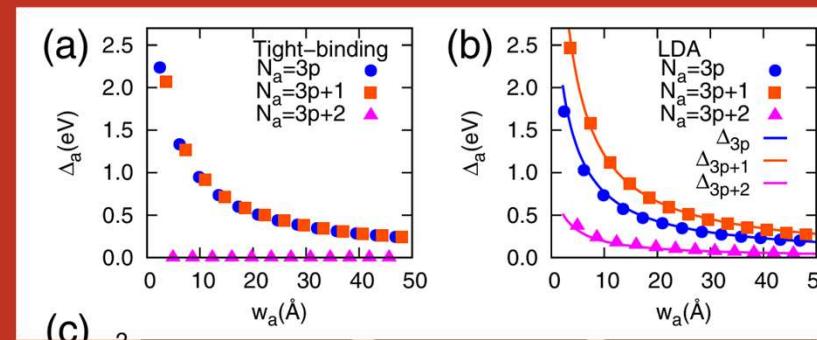
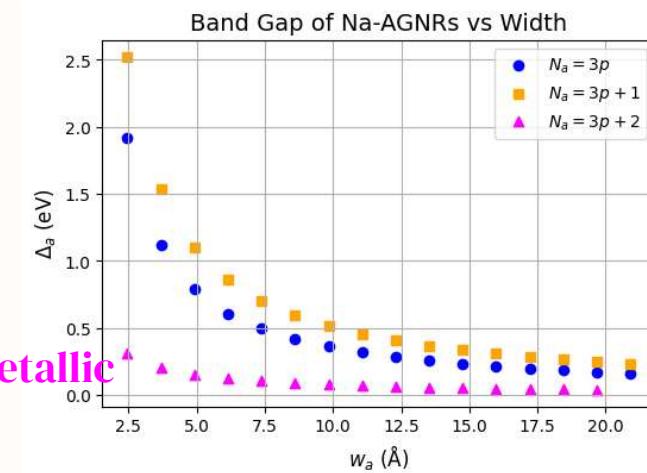
Band Gap as a Function of Width

$a = 1.42 \text{ \AA}$
 $t = 2.7 \text{ eV}$

No shrinking effect, $t = t_e$



Considering shrinking effect on the edge ($t_e = 1.12t$)



Son Y-W, Cohen M. L, and Louie S. G

Future Aspects

1. Compute zigzag graphene's band structure
2. Show ZGNRs' band gap as a function of width
3. Compare AGNRs and ZGNRs

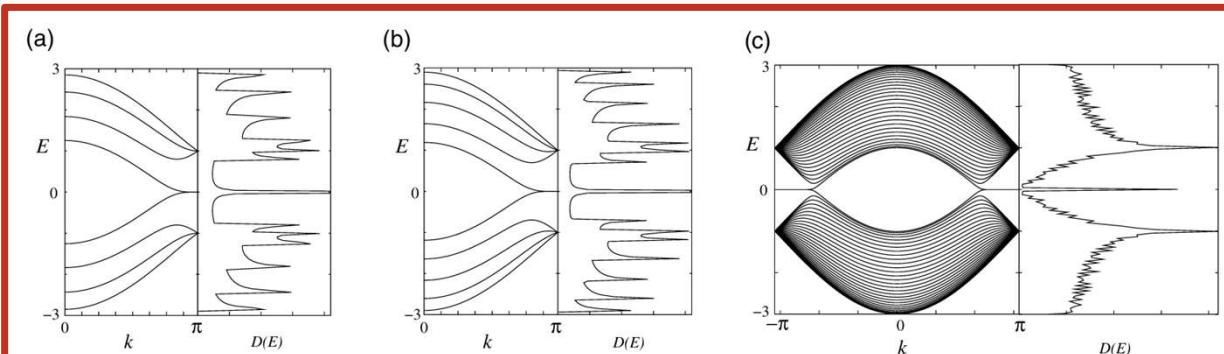
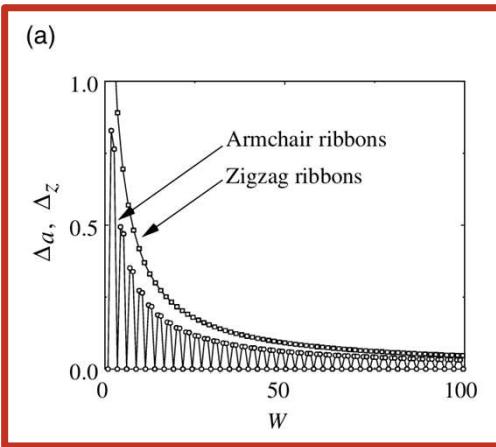


Figure 4. Energy band structure $E(k)$ and density of states $D(E)$ of zigzag ribbons of various widths: (a) $N = 4$, (b) $N = 5$ and (c) $N = 30$. Adapted from [89].

“

References

Son Y-W, Cohen M. L, and Louie S. G, Energy gaps in graphene nanoribbons, Phys. Rev. Lett. 97, 216803 (2006).

FranzUtermohlen. (2018, September 12). Tight-binding model for graphene. [Handout].

06.12 Tight binding theory - Band character and partial density of states

Wakabayashi, K., Sasaki, K. ichi, Nakanishi, T., & Enoki, T. (2010). Electronic states of graphene nanoribbons and analytical solutions. Science and Technology of Advanced Materials, 11(5). <https://doi.org/10.1088/1468-6996/11/5/054504>

Demo / Q&A Time.