Numerical Computations of Nanoelectronics Problems

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Outline
Three Lectures

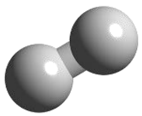
- Lecture on Tuesday
  - Numerical Calculation of Schrödinger Equation
    - 1D ∞ Quantum Well
  - Numerical Newton Iteration
    - Transcendental Equation (Capacitance of P-N Junction)
    - Poission's Equation (Band Diagram of P-N Junction)
- Lecture on Thursday
  - Numerical Calculation of Band Structures
    - 1D atom chain
    - Graphene Nanoribbon
    - Graphene
- Lecture in the final week
  - Quantum Transport – Non-equilibrium Green's Function

Band Structures
Tight-Binding Method

- H_2 molecule (Calculus of variations)

$$H_1\psi_1 = E_0\psi_1 \quad H_2\psi_2 = E_0\psi_2 \qquad H_i = -\frac{\hbar^2}{2m}\nabla^2 + V_i(r) \quad i = 1,2$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \sum_{i=1}^{2} V_i(r)$$



$$\psi = c_1\psi_1 + c_2\psi_2$$

Assume ψ_1 and ψ_2 are orthogonal

$$\int \psi_1^* H\psi d\tau = \int \psi_1^* E\psi d\tau = Ec_1$$

$$\int \psi_2^* H\psi d\tau = \int \psi_2^* E\psi d\tau = Ec_2$$

$$\alpha = E_0 = \int \psi_2^* H_2\psi_2 d\tau = \int \psi_1^* H_1\psi_1 d\tau$$

$$\beta = E_1 = \int \psi_2^* V_1\psi_2 d\tau = \int \psi_1^* V_2\psi_1 d\tau$$

$$\gamma = E_2 = \int \psi_2^* V_1\psi_1 d\tau = \int \psi_1^* V_2\psi_2 d\tau$$

$$H_{ij} = \int \psi_i^* H \psi_j \quad i,j = 1,2$$

$$H_{11} = \int \psi_1^* H \psi_1 d\tau = \int \psi_1^* (-\frac{\hbar^2}{2m} + V_1 + V_2) \psi_1 d\tau$$

$$= \int \psi_1^* (-\frac{\hbar^2}{2m} + V_1) \psi_1 d\tau + \int \psi_1^* V_2 \psi_1 d\tau$$

$$= \int \psi_1^* H_1 \psi_1 d\tau + \int \psi_1^* V_2 \psi_1 d\tau = E_0 + E_1 = \alpha + \beta$$

$$H_{12} = \int \psi_1^* H \psi_2 d\tau = \int \psi_1^* (-\frac{\hbar^2}{2m} + V_1 + V_2) \psi_2 d\tau$$

$$= \int \psi_1^* (-\frac{\hbar^2}{2m} + V_1) \psi_2 d\tau + \int \psi_1^* V_2 \psi_2 d\tau$$

$$= \int \psi_1^* H_1 \psi_2 d\tau + \int \psi_1^* V_2 \psi_2 d\tau = \int (H_1 \psi_1)^* \psi_2 d\tau + E_2$$

$$= \int (E_1 \psi_1)^* \psi_2 d\tau + \gamma = E_1 \int \psi_1^* \psi_2 d\tau + \gamma = 0 + \gamma = \gamma$$

$$H_{21} = \int \psi_2^* H \psi_1 d\tau = \int \psi_2^* (-\frac{\hbar^2}{2m} + V_1 + V_2) \psi_1 d\tau$$

$$= \int \psi_2^* (-\frac{\hbar^2}{2m} + V_2) \psi_1 d\tau + \int \psi_2^* V_1 \psi_1 d\tau$$

$$= \int \psi_2^* H_2 \psi_1 d\tau + \int \psi_2^* V_1 \psi_1 d\tau = \int (H_2 \psi_2)^* \psi_1 d\tau + E_2$$

$$= \int (E_2 \psi_2)^* \psi_1 d\tau + \gamma = E_2 \int \psi_2^* \psi_1 d\tau + \gamma = 0 + \gamma = \gamma$$

$$H_{22} = \int \psi_2^* H \psi_2 d\tau = \int \psi_2^* (-\frac{\hbar^2}{2m} + V_1 + V_2) \psi_2 d\tau$$

$$= \int \psi_2^* (-\frac{\hbar^2}{2m} + V_2) \psi_2 d\tau + \int \psi_2^* V_1 \psi_2 d\tau$$

$$= \int \psi_2^* H_2 \psi_2 d\tau + \int \psi_2^* V_1 \psi_2 d\tau = E_0 + E_1 = \alpha + \beta$$

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = \begin{bmatrix} \alpha + \beta & \gamma \\ \gamma & \alpha + \beta \end{bmatrix}$$

$$H = \begin{bmatrix} \alpha + \beta & \gamma \\ \gamma & \alpha + \beta \end{bmatrix} \qquad \psi = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

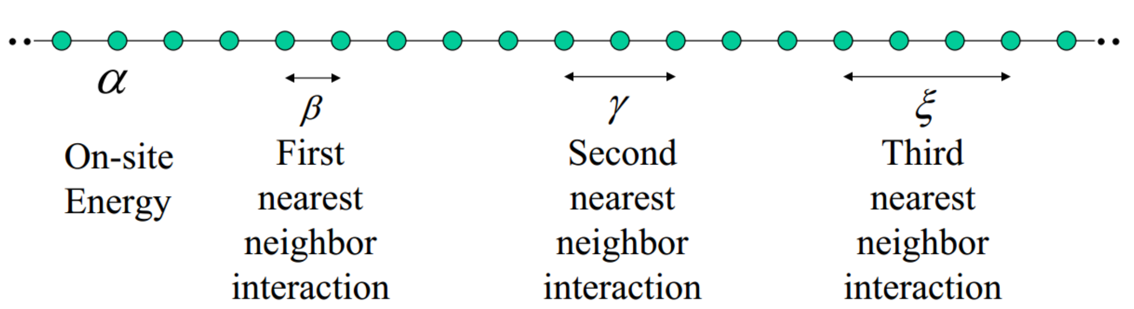
$$\begin{bmatrix} \alpha + \beta & \gamma \\ \gamma & \alpha + \beta \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

```
alpha=-13.6;
beta=0;
gamma=1.7;

H=
[ alpha+beta  gamma      ;
 gamma      alpha+beta ];

[V,E]=eig(H);
```

−15.3eV −11.9eV

Band Structures
Tight-Binding Method

- TB description for 1D chain of atoms

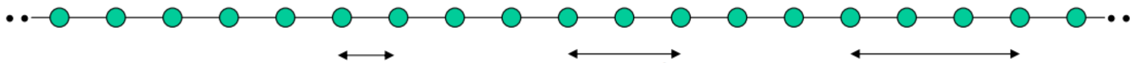


$$H = \begin{bmatrix} \alpha & \beta & \gamma & \xi & . \\ \beta^{+} & \alpha & \beta & \gamma & . \\ \gamma^{+} & \beta^{+} & \alpha & \beta & . \\ \xi^{+} & \gamma^{+} & \beta^{+} & \alpha & . \\ . & . & . & . & \dots \end{bmatrix}$$

In solid-state physics, the tight-binding model (or TB model) is an approach to the calculation of electronic band structure using an approximate set of wave functions based upon superposition of wave functions for isolated atoms located at each atomic site.

Band Structures
Tight-Binding Method

- First Nearest Neighbor TB Description

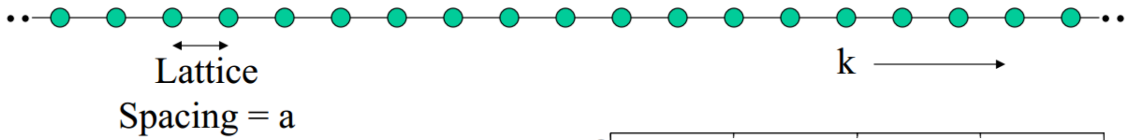


$\alpha = E_{bo} + 2t_o$ $\beta = -t_o$ $\gamma = 0$ $\xi = 0$

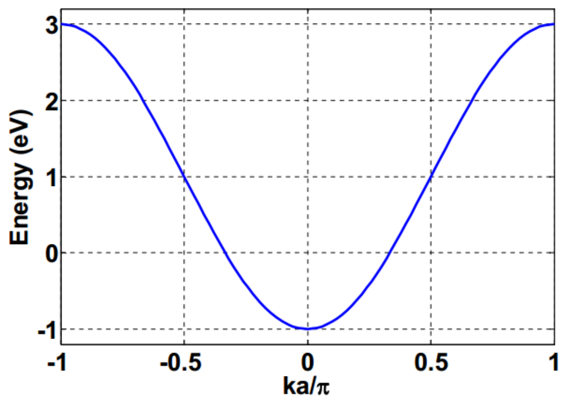
$$H = \begin{bmatrix} E_{bo}+2t_o & -t_o & 0 & 0 & . \\ -t_o & E_{bo}+2t_o & -t_o & 0 & . \\ 0 & -t_o & E_{bo}+2t_o & -t_o & . \\ 0 & 0 & -t_o & E_{bo}+2t_o & . \\ . & . & . & . & \cdots \end{bmatrix}$$

Band Structures
Tight-Binding Method

- First Nearest Neighbor TB Description – E(k)



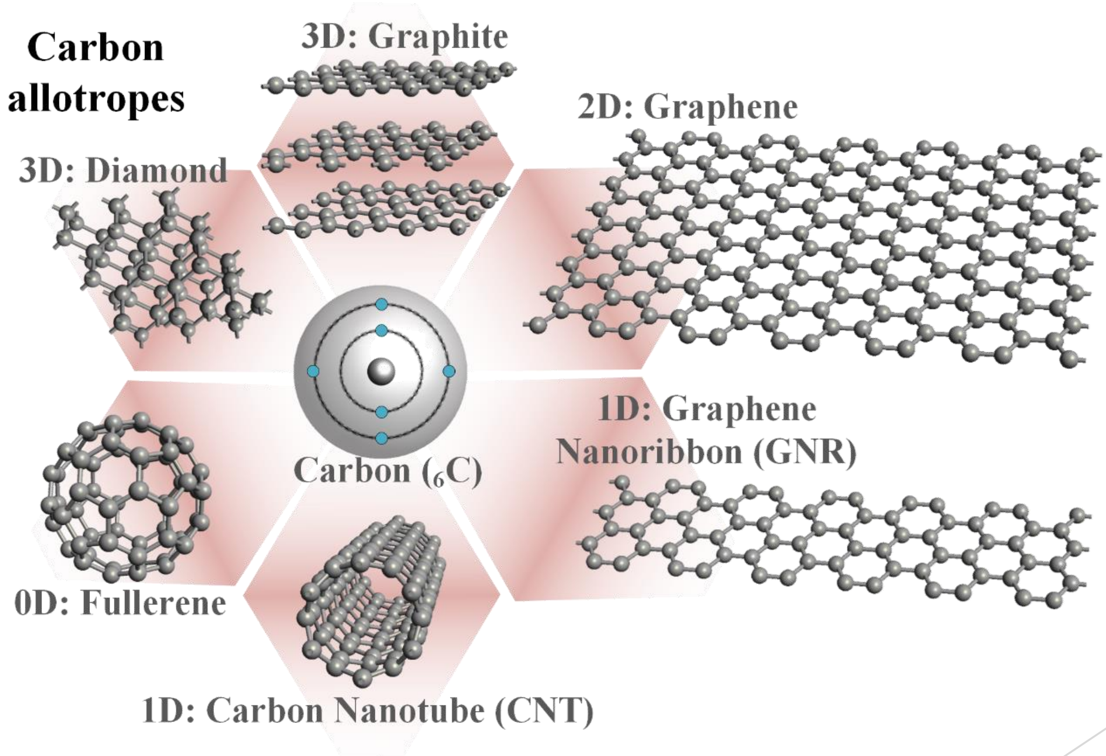
$$E(k) = \sum_{m=1}^{N} H_{mn} e^{i\vec{k}.(\vec{d_m}-\vec{d_n})}$$
$$= E_{bo} + 2t_o - t_o e^{ika} - t_o e^{-ika}$$
$$= E_{bo} + 2t_o - t_o\left[e^{ika} + e^{-ika}\right]$$
$$= E_{bo} + 2t_o\left[1 - \cos(ka)\right]$$



- Applications:
  - effective mass model for various materials
  - pz-orbital tight binding model for CNTs and GNRs.

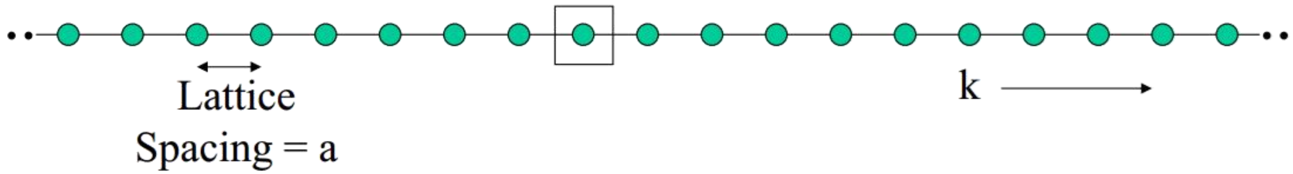
Band Structures
Tight-Binding Method

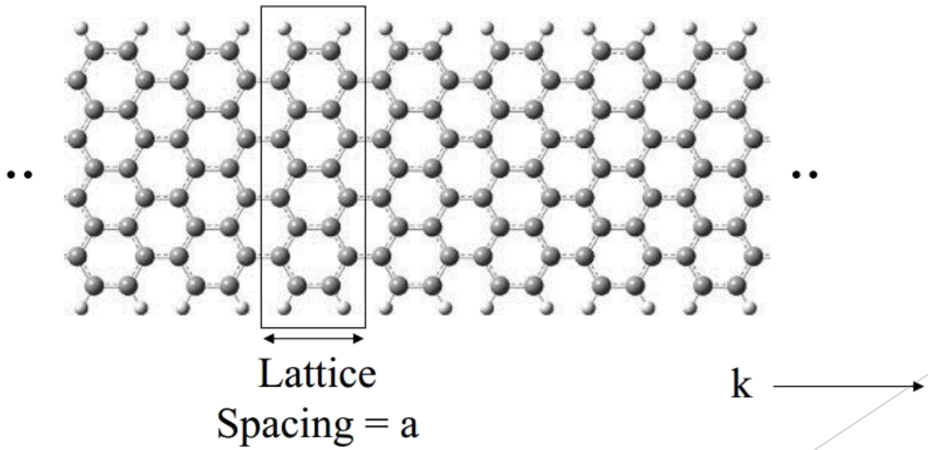
- Graphene Nanoribbon



Band Structures
Tight-Binding Method

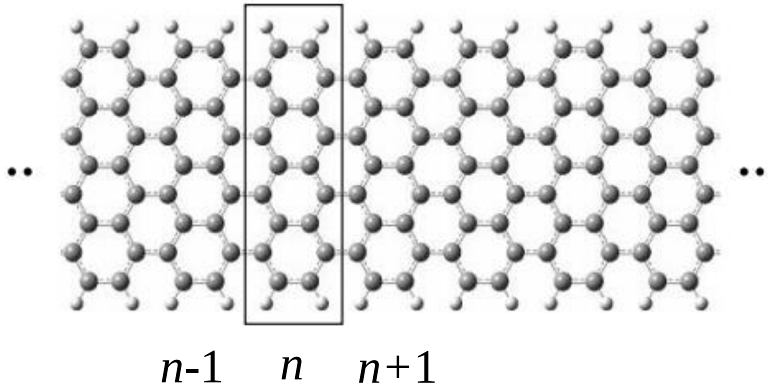
- Problem: Band structure of GNR





Band Structures
Tight-Binding Method

- $$E(k) = \sum_{m=1}^{N} H_{mn} e^{i\vec{k}.(\vec{d_m} - \vec{d_n})}$$



$$H_{n,n}$$

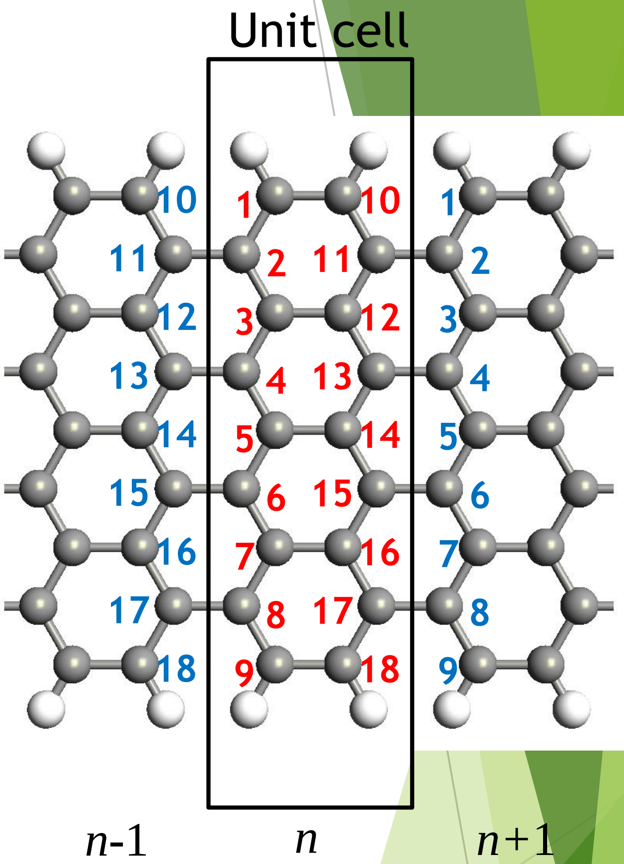
$$H_{n,n+1}$$

$$H_{n,n-1}$$

- Hamiltonian

$H_{nn} =$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1		t								t								
2	t		t															
3		t		t								t						
4			t		t													
5				t		t								t				
6					t		t											
7						t		t								t		
8							t		t									
9								t										t
10	t										t							
11										t		t						
12			t								t		t					
13												t		t				
14					t								t		t			
15														t		t		
16							t								t		t	
17																t		t
18									t								t	




```
t=-2.7;
Hnn_ul=diag(ones(8,1),1)+diag(ones(8,1),-1);
Hnn_br=diag(ones(8,1),1)+diag(ones(8,1),-1);
Hnn_ur=diag([1 0 1 0 1 0 1 0 1]);
Hnn_bl=diag([1 0 1 0 1 0 1 0 1]);
Hnn=t*[Hnn_ul Hnn_ur; Hnn_bl Hnn_br];
```

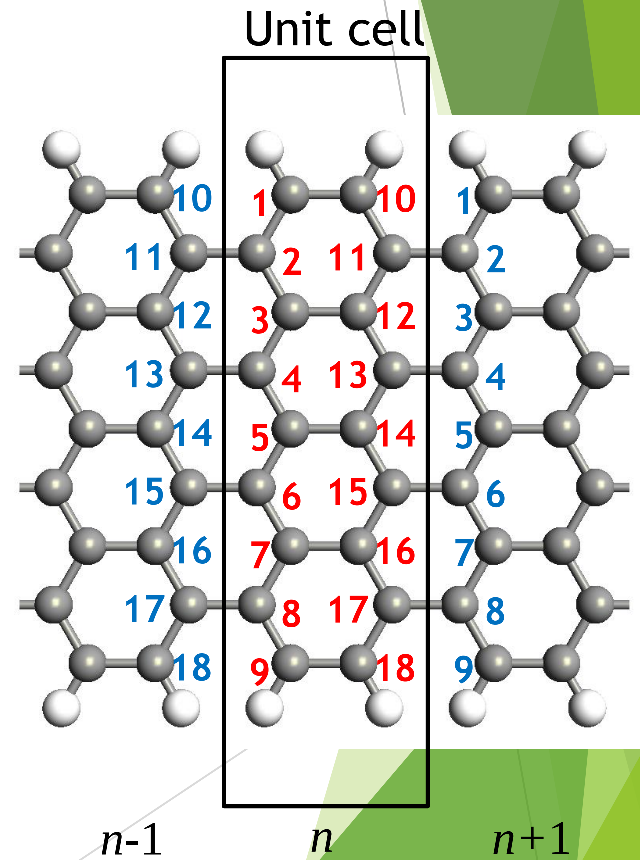
Band Structures
Tight-Binding Method

- Hamiltonian

$H_{n,n+1} =$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1																		
2																		
3																		
4																		
5																		
6																		
7																		
8																		
9																		
10																		
11		t																
12																		
13				t														
14																		
15						t												
16																		
17								t										
18																		

```
Hnm=t*diag([0 1 0 1 0 1 0 1 0], 9);
```



Band Structures
Tight-Binding Method

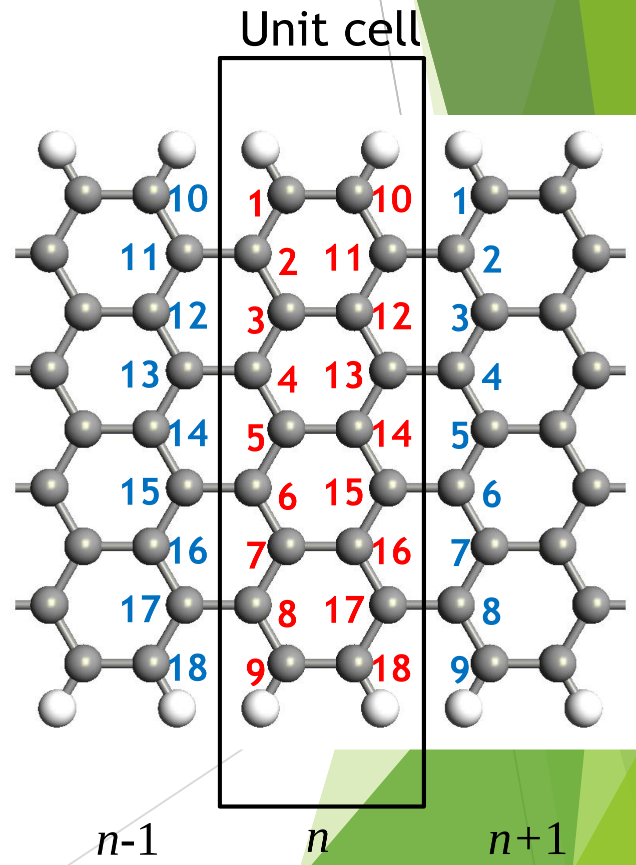
- Hamiltonian

$H_{n,n-1}$ =

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1																		
2											t							
3																		
4													t					
5																		
6															t			
7																		
8																	t	
9																		
10																		
11																		
12																		
13																		
14																		
15																		
16																		
17																		
18																		

```
Hmn=t*diag([0 1 0 1 0 1 0 1 0], -9);
```

transpose of $H_{n,n+1}$



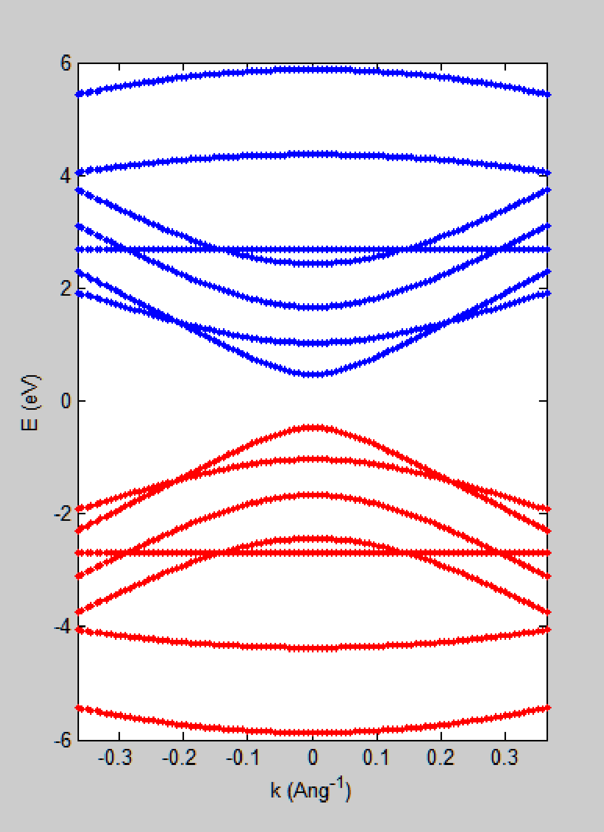
Band Structures
Tight-Binding Method

- Hamiltonian:

$$\sum_{m=1}^{N} H_{mn} e^{i\vec{k}.(\vec{d}_m - \vec{d}_n)}$$

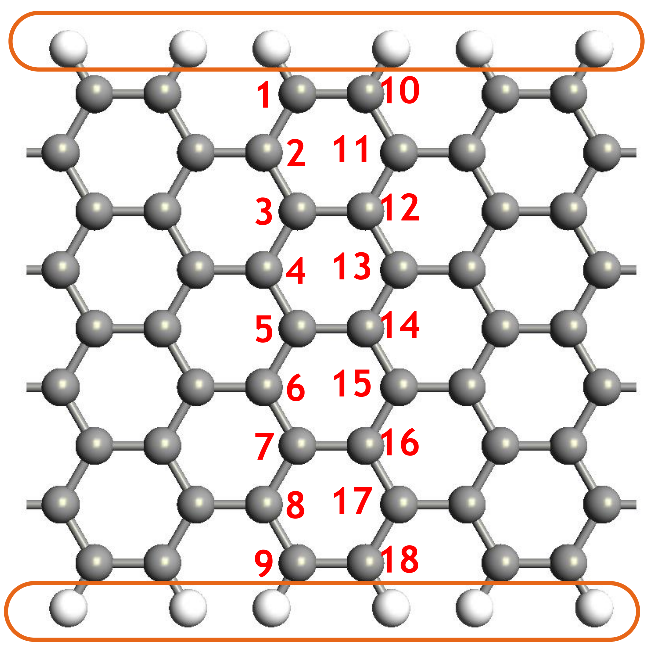
$$= H_{nn} + H_{n,n+1}e^{-ika} + H_{n,n-1}e^{ika}$$

```
hold on; box on;
a=3*1.44;
k_grid=linspace(-pi/2/a,pi/2/a,101);
for k=k_grid
    H=Hnn+Hnm*exp(-1i*k*a)+Hmn*exp(1i*k*a);
    [V E]=eig(H);
    E=diag(E);
    plot(k,E(1:9),'r.');
    plot(k,E(10:18),'b.');
end
axis tight
ylim([-6 6]);
xlabel('k (Ang^{-1})');
ylabel('E (eV)');
```



Band Structures
Tight-Binding Method

- Considering hydrogen atoms at edges…

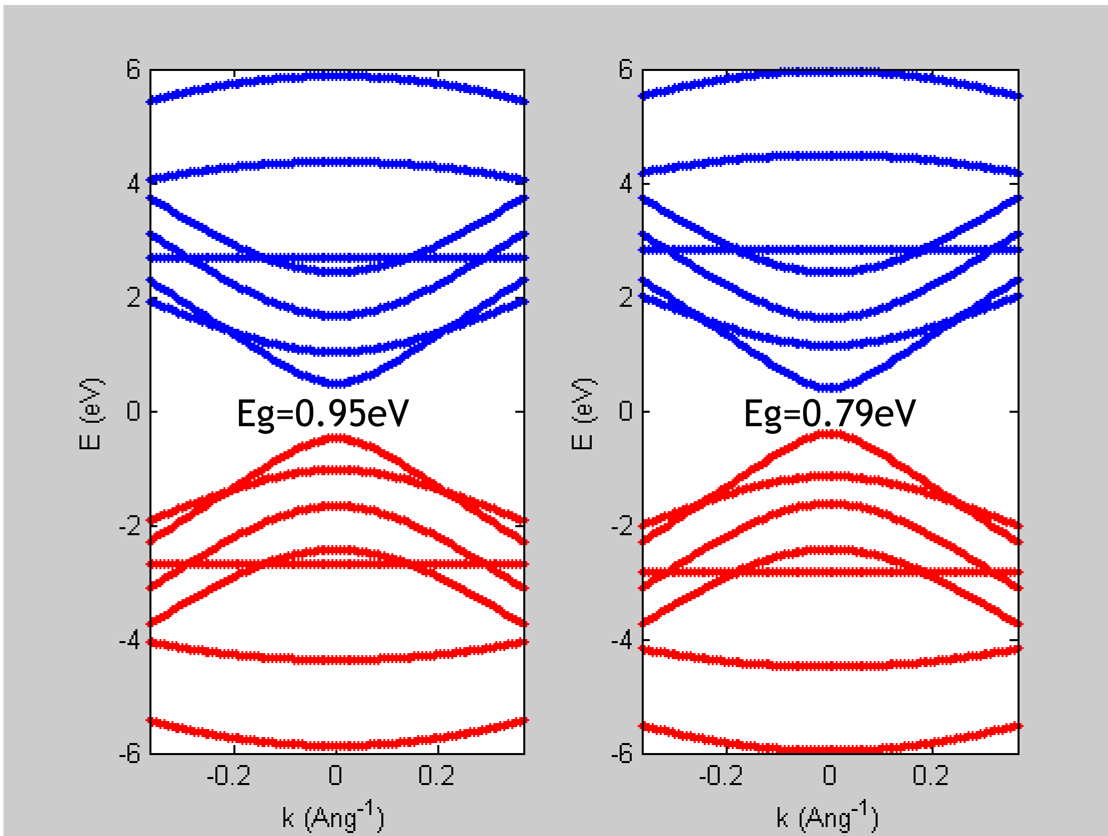


$H_{nn} =$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1		t								$t \times 1.12$								
2	t		t															
3		t		t								t						
4			t		t													
5				t		t								t				
6					t		t											
7						t		t								t		
8							t		t									
9								t										$1.12 \times t$
10	$t \times 1.12$										t							
11										t		t						
12			t								t		t					
13												t		t				
14					t								t		t			
15														t		t		
16							t								t		t	
17																t		t
18									$t \times 1.12$								t	

```
Hnn_ur=diag([1.12 0 1 0 1 0 1 0 1.12]);
Hnn_bl=diag([1.12 0 1 0 1 0 1 0 1.12]);
```

Band Structures
Tight-Binding Method

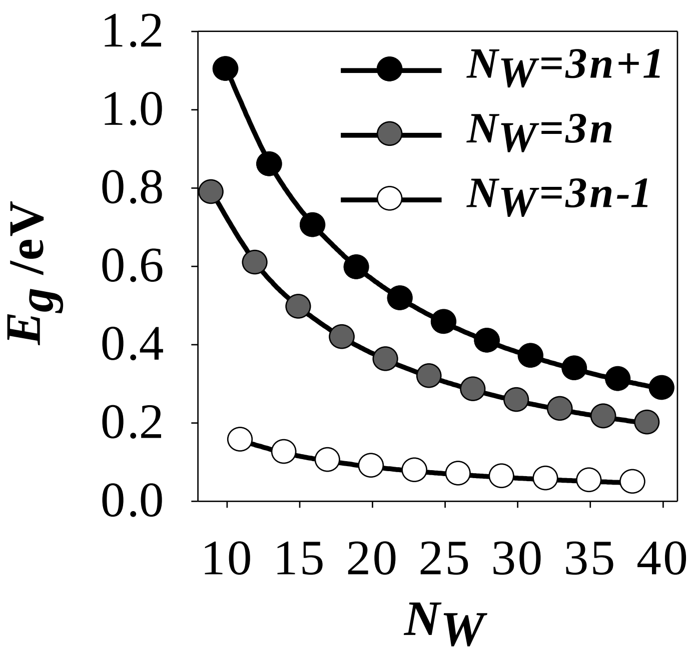


Unsaturated | Hydrogen saturated

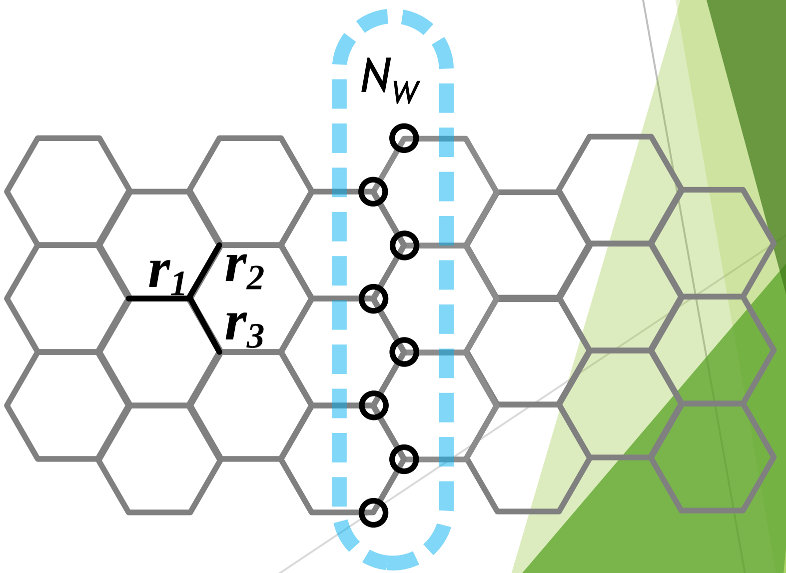
$m=0.092m_0$ | $m=0.075m_0$

Band Structures
Tight-Binding Method

- Armchair GNR Band gap – TB Results

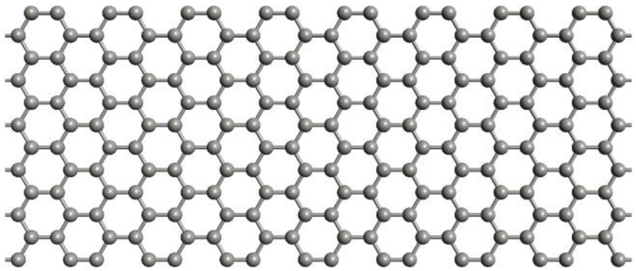


N_W=number of C atom along width

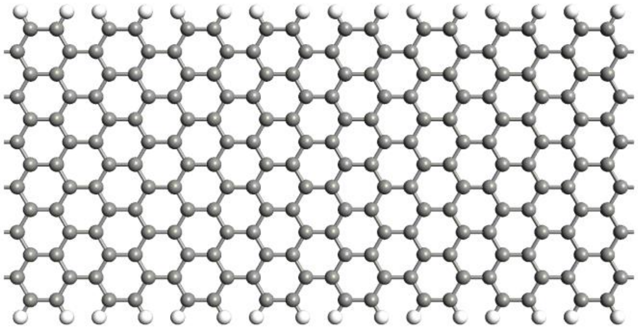


Band Structures
Tight-Binding Method

- Assignment 2, Problem 4:
- Calculate GNR band structure for:



N_W=12 unsaturated edge



N_W=13 saturated edge

Band Structures
Tight-Binding Method

- Band structure of graphene?

$$H = H_{nn} + H_{n,n1}e^{-i\vec{k}\overrightarrow{a1}} + H_{n,n2}e^{-i\vec{k}\overrightarrow{a2}} + H_{n,n3}e^{-i\vec{k}\overrightarrow{a3}} + H_{n,n4}e^{-i\vec{k}\overrightarrow{a4}}$$

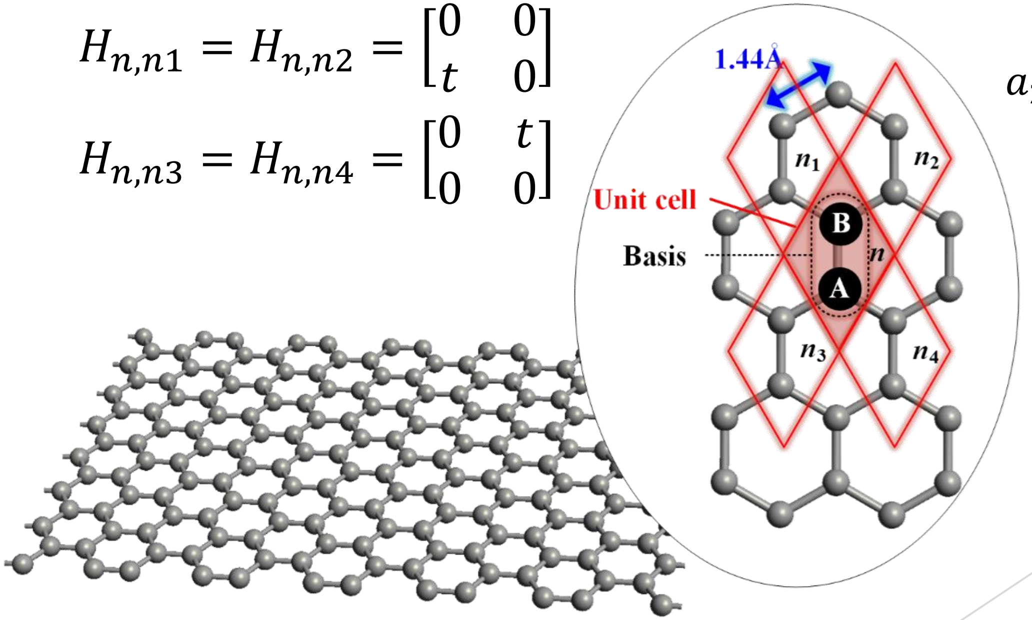
$$H_{nn} = \begin{bmatrix} 0 & t \\ t & 0 \end{bmatrix}$$

$$a_1 = -a_3 = 1.44\text{Å} \times \left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right)$$

$$H_{n,n1} = H_{n,n2} = \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix}$$

$$a_2 = -a_4 = 1.44\text{Å} \times \left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)$$

$$H_{n,n3} = H_{n,n4} = \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix}$$



Band Structures
Tight-Binding Method

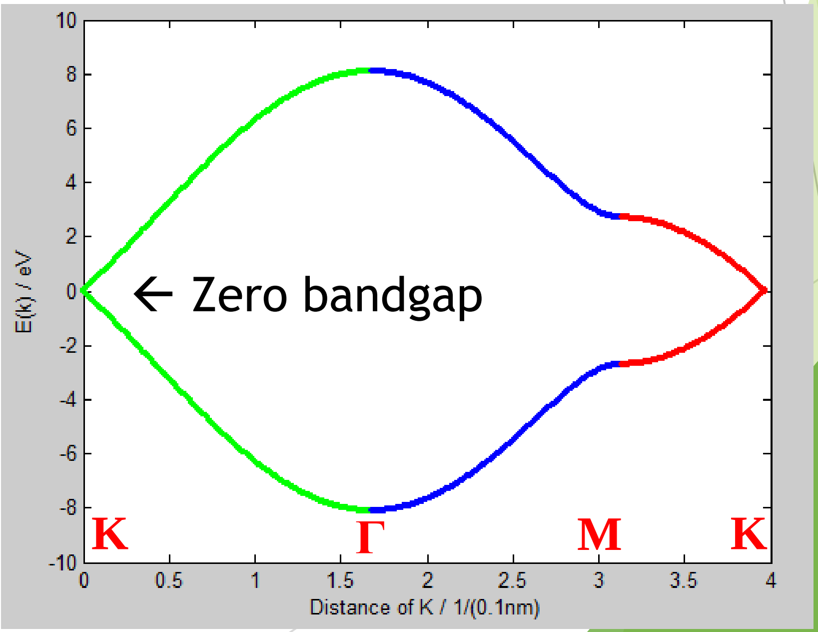
- Solve *H* in MATLAB along the route **K-Γ-M-K**

$$k=(0\,,0\,,0)\qquad k=(\frac{2\pi}{3a_{cc}}\,,0\,,0)\qquad k=(\frac{2\pi}{3a_{cc}}\,,\frac{2\pi}{3\sqrt{3}a_{cc}}\,,0)$$

Symmetric point **Γ** in k space

K

M



Band Structures
Tight-Binding Method

- Solve in k plane:
- Assignment 2 Bonus Problem: plot this figure using MATLAB