
Introduction to CNTbands

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Introduction to CNTbands

Description of the CNTbands Simulator

- Computes Electronic Band Structure for Carbon Nanotubes:
 - Molecular Structure (with graphical view)
 - Bandstructure
 - Density of States

CNTbands was written in 2002 by J. Guo of Purdue University. It is based on a script by M. P. Anantram of NASA Ames Research Center and the paper, L. Yang, M. P. Anantram, and J. P. Lu, "Band-gap change of carbon nanotubes: Effect of small uniaxial and torsional strain," *Physical Review B*, vol. 60, no. 29, pp. 13874-13878, 1999.

Introduction to CNTbands

Description of the CNTbands Examples

- Example 1: Atomistic Structure of CNTs
- Example 2: Properties of Armchair CNTs
- Example 3: Properties of Zigzag CNTs
- Example 4: Dependence of Material Properties on the CNT Diameter

Exercise 1 – Atomistic Structure

A (m, n) CNT can be simulated using CNTbands by inputting m and n ,

(a) simulate a $(7,7)$ CNT and print out its unit cell structure. Why are CNTs with $m=n$ called armchair CNTs? What is the length of a unit cell?

(b) simulate a $(13,0)$ CNT and print out its unit cell structure. Why are CNTs with $n=0$ called zigzag CNTs? What is the length of a unit cell?

(c) Simulate a $(10,7)$ CNT, What is the length of a unit cell?

(d) Read T in Table 3.3 in Physical Properties of Carbon Nanotubes by Saito to compute the length of a unit cell for (a)-(c). How do the computed results compare to the simulation results?

1a) (7,7) CNT

Parameters and Settings

The screenshot shows a software interface for simulating a Carbon Nanotube (CNT). The main section is titled "Parameters and Settings". At the top right, there is a yellow bar with a "Simulate" button and the text "new input parameters". Below this is a "Result:" label and a dropdown menu. The central part of the interface is a large grid area, currently empty, with a "No results" message and a "Clear" button at the bottom right. On the left side, there are several input fields:

- Chirality (n, m):** Two input fields, "n: 7" and "m: 7", are circled in red. Each field has up and down arrow buttons to its right.
- Model parameters:**
 - Tight Binding Energy: 3eV (with a blue icon)
 - Carbon-carbon spacing: 1.42Å (with a yellow icon)
 - Length of nanotube in 3-D view: 15 (with up and down arrow buttons)

At the bottom left, there are two buttons: "Refresh Screen" and "Copy/Paste with Desktop".

1a) (7,7) CNT

Unit Cell Structure

Simulate

Result: Molecular structure: unit cell

Chirality (n,m)

n: 7

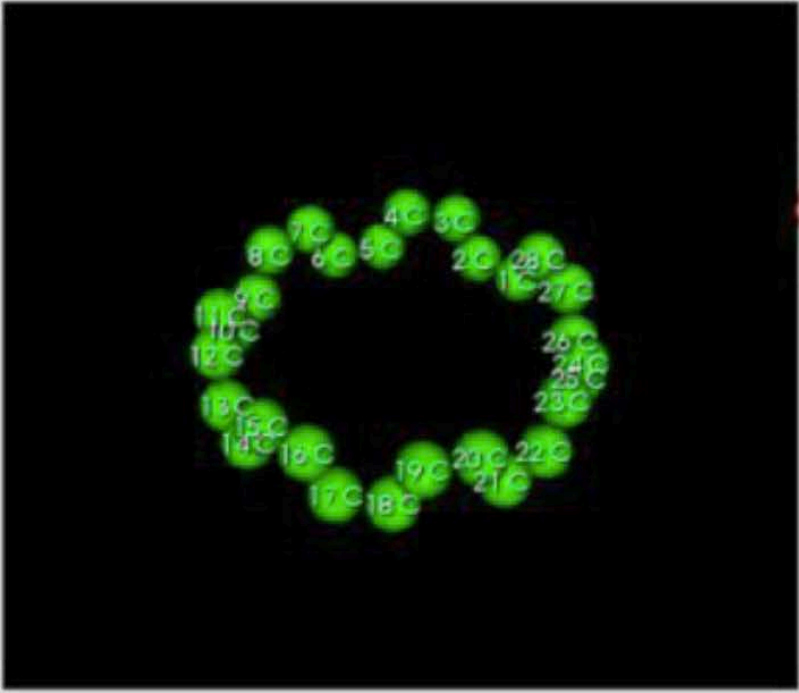
m: 7

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42Å

Length of nanotube in 3-D view: 15



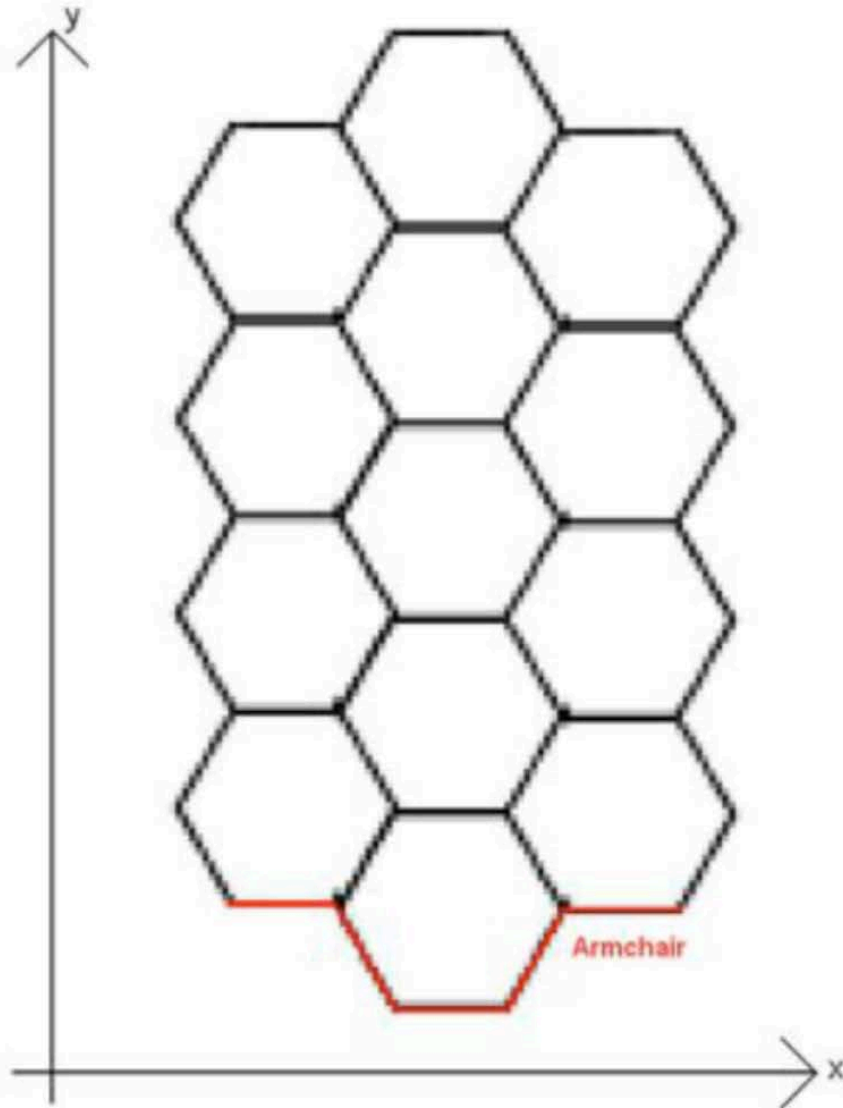
1 result

Clear

Refresh Screen | Copy/Paste with Desktop

1a) (7,7) CNT

Nomenclature: Armchair



1a) (7,7) CNT

Unit Cell Length for (7,7) CNT: 0.24595nm

The screenshot displays a simulation software interface for a (7,7) carbon nanotube. The interface includes a 'Simulate' button at the top. Below it, a 'Result' dropdown menu is set to 'Output Log'. The main display area shows the following parameters:

- Nanotube diameter (nm): 0.94920
- Nanotube circumference (nm): 12.124
- Chiral angle (degrees): 30.000
- Length of unit cell (nm): 0.24595 (highlighted with a red circle and a mouse cursor)
- Number of hexagons (unit cell): 14
- DOS Energy Range (eV) [-x : x]: 3.7300
- Boundary of Brillouin Zone (ktaax): 1.2773e+10
- Bandgap Magnitude (eV):

On the left side, the 'Chirality (n,m)' section shows n: 7 and m: 7. The 'Model parameters' section includes:

- Tight Binding Energy: 3eV
- Carbon-carbon spacing: 1.42A
- Length of nanotube in 3-D view: 15

At the bottom, there is a 'Find:' search bar, a 'Select All' button, and a 'Clear' button. The status bar at the very bottom shows '1 result' and 'Refresh Screen | Copy/Paste with Desktop'.

1b) (13,0) CNT

Unit Cell Structure

Simulate

Result: Molecular structure: unit cell

Chirality (n,m)

n: 13

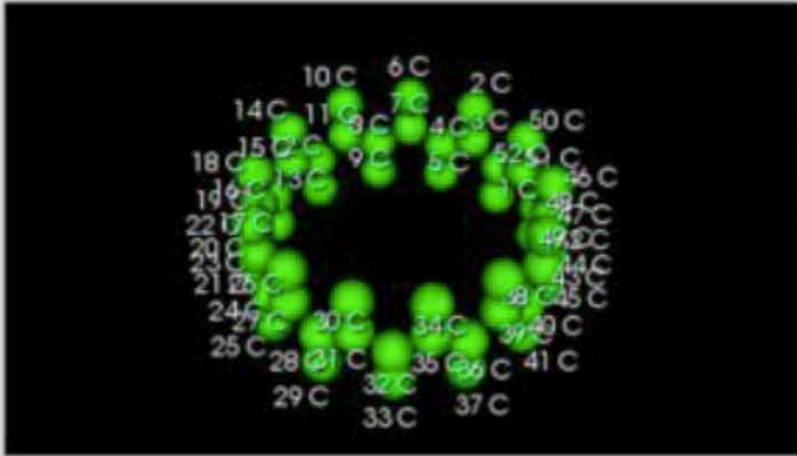
m: 0

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42Å

Length of nanotube in 3-D view: 15



2 results Clear

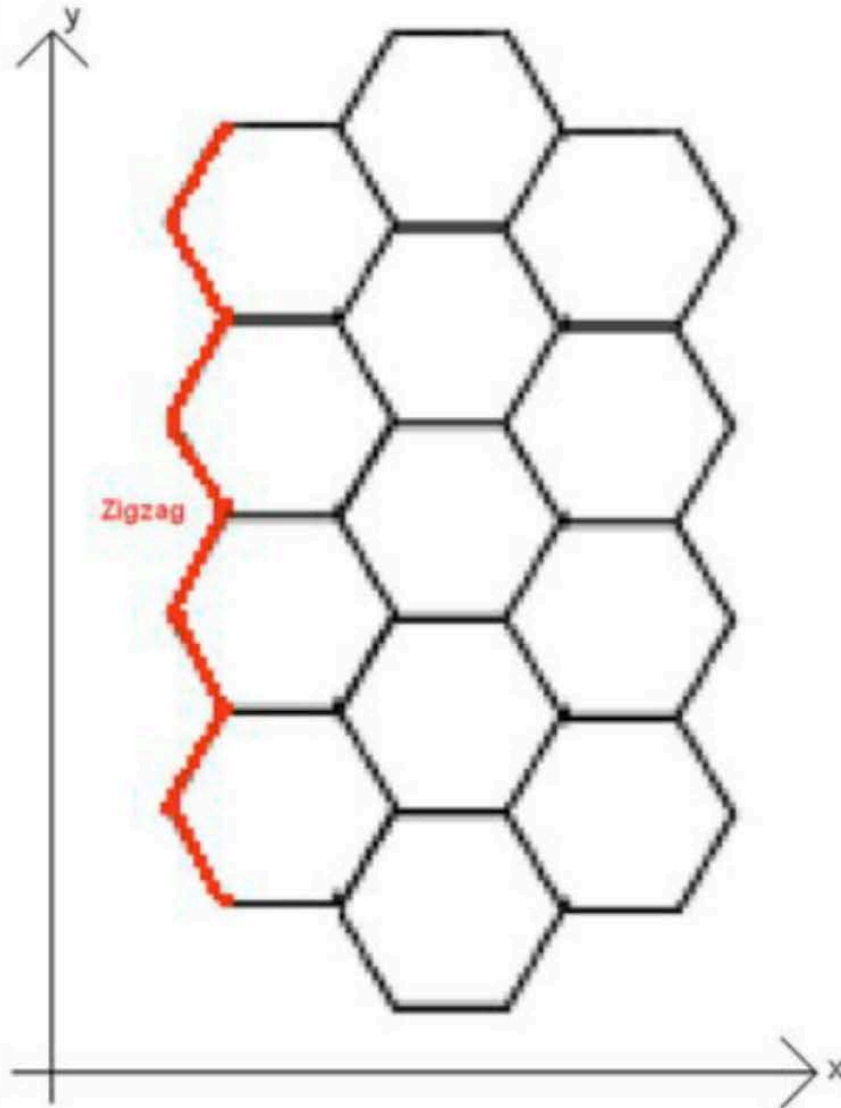
All n 13

All m 0

Refresh Screen Copy/Paste with Desktop

1b) (13,0) CNT

Nomenclature: Zigzag



1b) (13,0) CNT

Unit Cell Length for (13,0) CNT: 0.426nm

The screenshot displays a simulation interface for a (13,0) Carbon Nanotube (CNT). On the left side, there are input fields for Chirality (n,m), Model parameters, and Length of nanotube in 3-D view. The Chirality (n,m) section shows n: 13 and m: 0. The Model parameters section shows Tight Binding Energy: 3eV and Carbon-carbon spacing: 1.42A. The Length of nanotube in 3-D view is set to 15. On the right side, there is a 'Simulate' button and a 'Result' dropdown menu set to 'Output Log'. The output log displays the following results:

- Nanotube circumference (nm): 13.000
- Chiral angle (degrees): 0
- Length of unit cell (nm): 0.42600
- Number of hexagons (unit cell): 26
- DOS Energy Range (eV) [-x : x]: 2 n1n1

The 'Length of unit cell (nm)' result is highlighted with a red oval and a mouse cursor. Below the output log, there is a 'Find' search bar and a 'Select All' button. At the bottom, there are two sliders for 'n' and 'm', both set to their respective values (13 and 0). The interface also shows '2 results' and a 'Clear' button.

1d) Unit Cell Length

The referenced equation is:

$$T = \frac{\sqrt{3} \cdot L}{d_R}$$

$$L = 2.46 \text{ \AA} \cdot \sqrt{n^2 + m^2 + n \cdot m}$$

$$d_R = \text{gcd}(2n + m, 2m + n)$$

1d) Unit Cell Length

Results:

(m,n)	Simulated Unit Length (nm)	Computed Unit Length (nm)
(7,7)	0.24595	0.246
(13,0)	0.42600	0.426
(10,7)	2.10140	2.102

Exercise 2 – Armchair CNTs

Simulate a (7, 7) CNT and answer the following questions

(a) Is the CNT metallic or semiconducting? How many valleys are there in a Brillouin zone?

(b) Use zone-folding method to explain why armchair CNTs are always metallic.

(c) What is the carrier velocity near the Fermi level?

(d) What is the simulated density of states near the Fermi level? How

does it compare to the computed value, $D(E) = \frac{4}{\pi \hbar v_F}$?

2a) Conduction of (7,7) CNT

Parameters and Settings

Simulate new input parameters

Result:

Chirality (n,m)

n: 7

m: 7

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

Length of nanotube in 3-D view: 15

No results

Clear

Refresh Screen | Copy/Paste with Desktop

2a) Conduction of (7,7) CNT

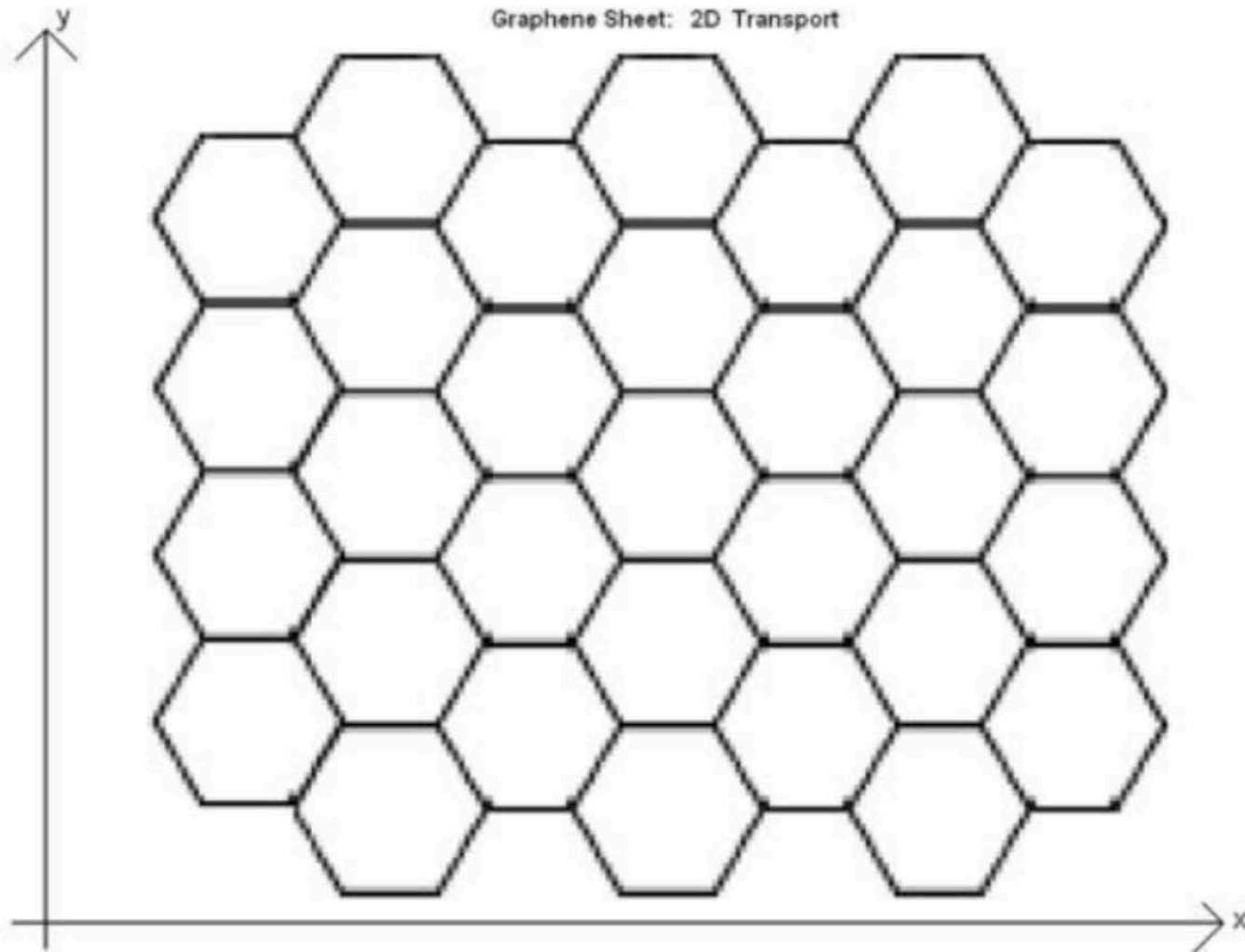
Energy Band Structure

The screenshot displays a simulation window for a (7,7) Carbon Nanotube (CNT). The interface is divided into several sections:

- Chirality (n,m):** n: 7, m: 7
- Model parameters:**
 - Tight Binding Energy: 3eV
 - Carbon-carbon spacing: 1.42Å
 - Length of nanotube in 3-D view: 15
- Simulation Results:**
 - Length of unit cell (nm): 0.24595
 - Number of hexagons (unit cell): 14
 - DOS Energy Range (eV) [-x : x]: 3.7300
 - Boundary of Brillouin Zone (ktaax): 1.2773e+10
 - Bandgap Magnitude (eV): 0.054496** (highlighted with a red circle and a mouse cursor)
 - Bandgap Magnitude in units of overlap parameter (t): 0.018165
 - kt at bandgap: -0.67000
- Search and Navigation:** Find: [] [down] [up] Select All
- Status:** 1 result Clear
- Footer:** Refresh Screen | Copy/Paste with Desktop

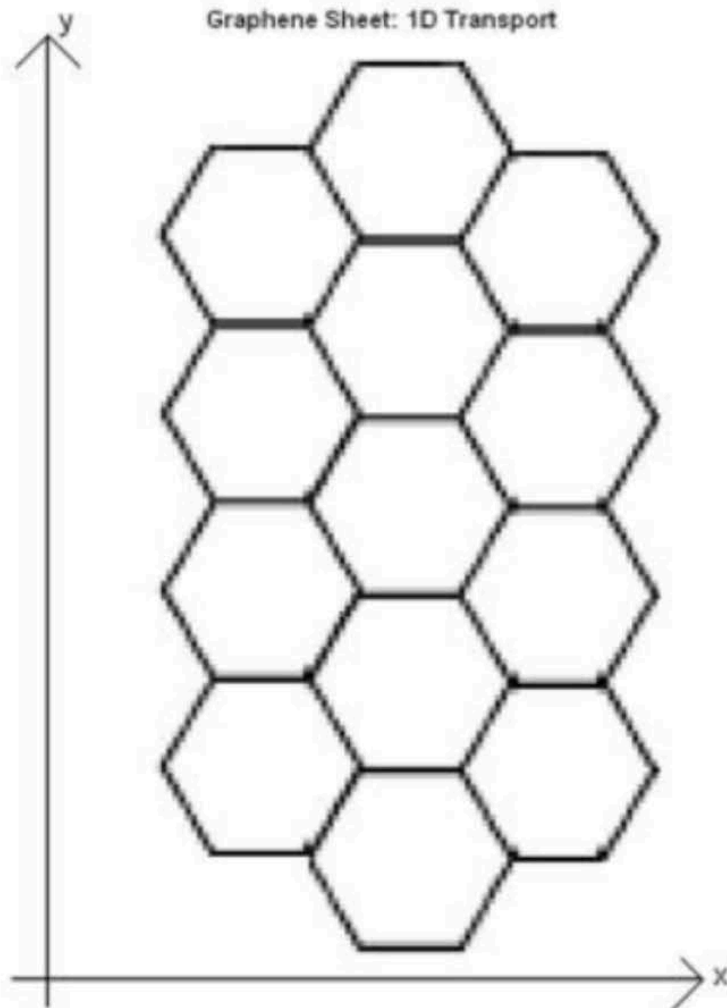
2b) Zone-Folding Method

Zone-Folding Method: Metallic Property of Armchair CNTs



2b) Zone-Folding Method

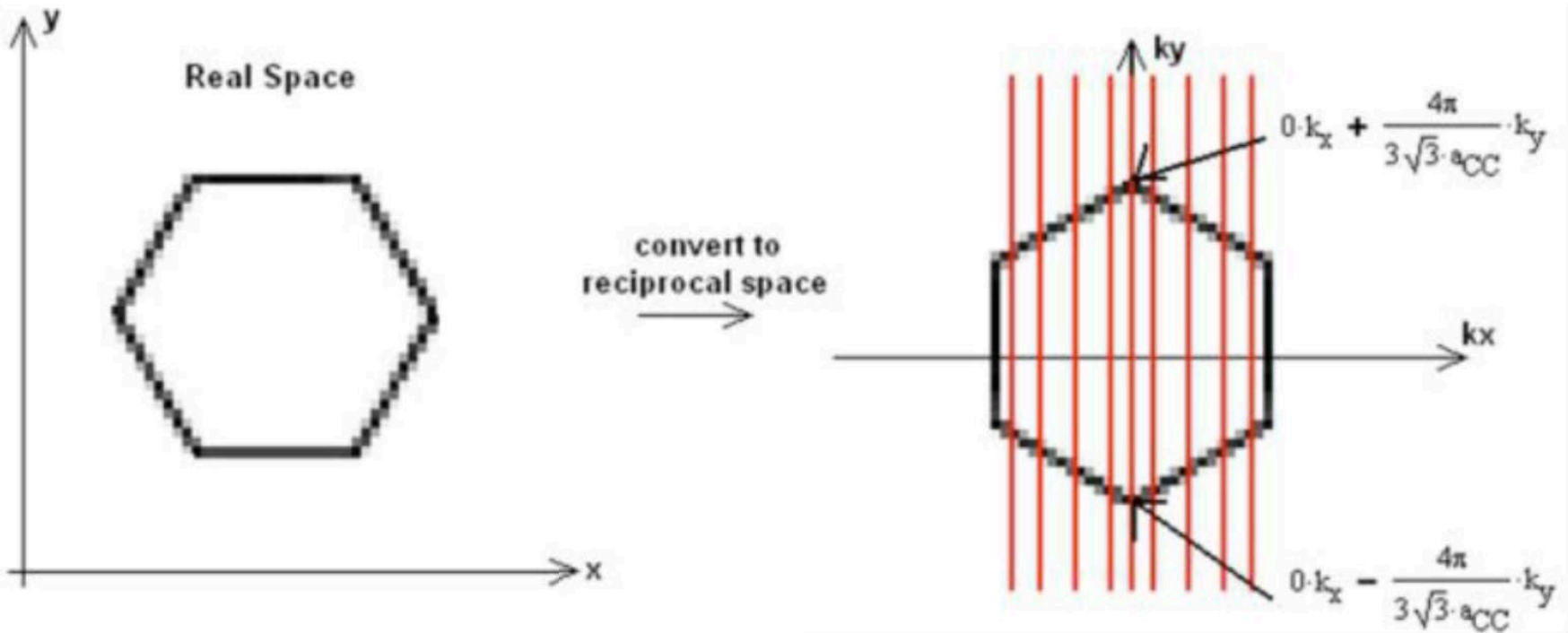
Zone-Folding Method: Metallic Property of Armchair CNTs



2b) Zone-Folding Method

Zone-Folding Method: Metallic Property of Armchair CNTs

Graphene Fermi Points: $0 \cdot k_x \pm \frac{4\pi}{3\sqrt{3} a_{CC}} \cdot k_y$



2c) Carrier Velocity

Computing v_F :

$$v_F = \frac{1}{\hbar} \cdot \frac{dE}{dk}$$

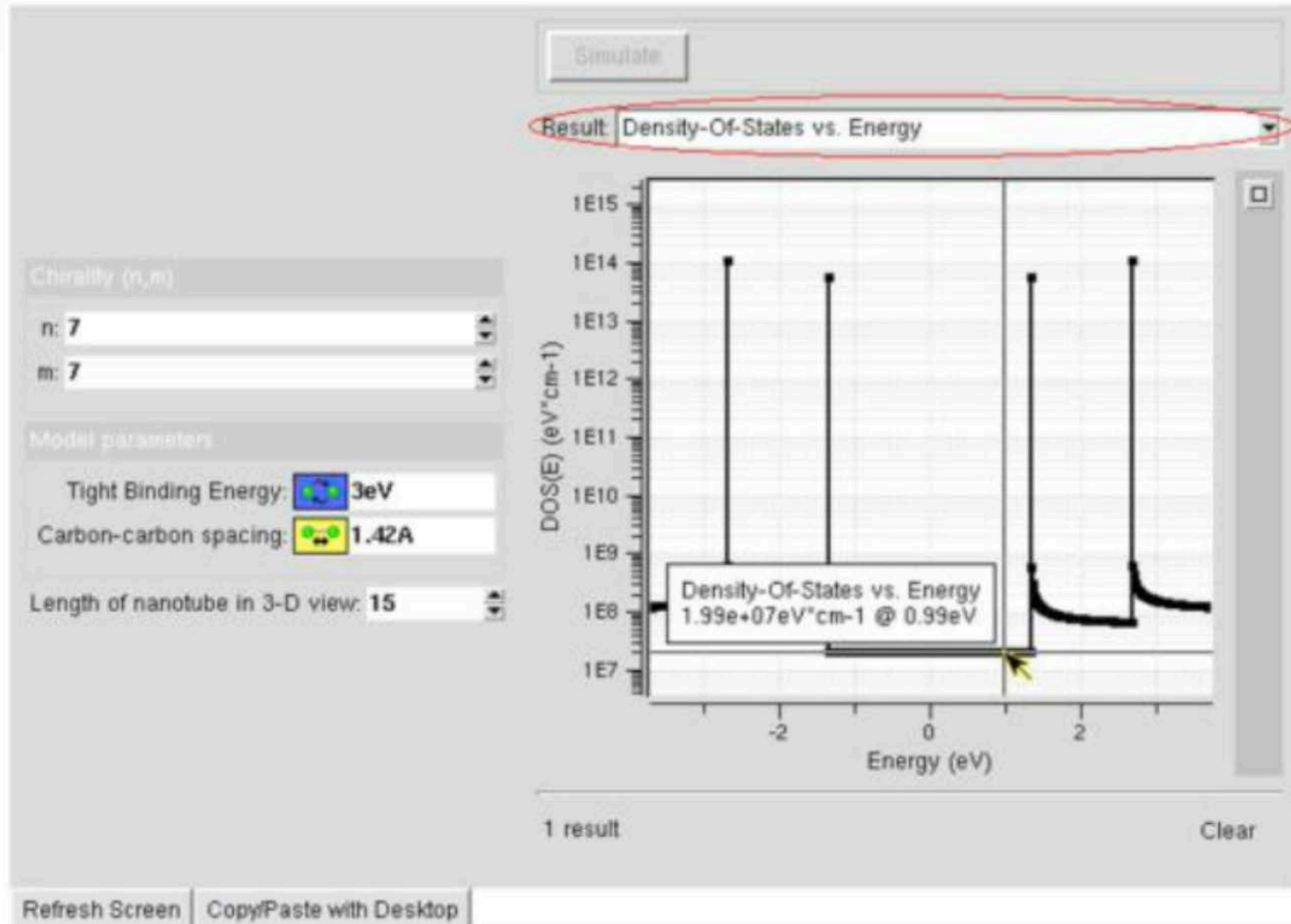
$$k_{tmax} = \frac{\pi}{\sqrt{3} \cdot a_{CC}} \quad a_{CC} = 1.42 \text{Ang}$$

$$k_{tmax} = 1.28 \text{E}8 \text{cm}^{-1}$$

$$\frac{dE}{dk} = 6.71 \text{E}-8 \text{cm} \cdot \text{eV}$$

$$v_F = 1.0 \text{E}8 \cdot \frac{\text{cm}}{\text{s}}$$

2d) DOS near Fermi Level



2d) DOS near Fermi Level

DOS at Fermi Level Simulation Result: 1.99E7/eVcm

Computed Value:

$$D(E) = \frac{4}{\pi \hbar v_F}$$

$$v_F = 1.0E8 \cdot \frac{\text{cm}}{\text{s}}$$

$$D(E) = 1.93E7 \cdot (\text{cm} \cdot \text{eV})^{-1}$$

Exercise 3 – Zigzag CNTs

Simulate a (13,0) CNT and answer the following questions,

(a) Is the CNT metallic or semiconducting? If semiconducting, what's the band gap of the lowest subband?

(b) Plot the density-of-states, why does it show singularities at the subband gaps?

Hint: DOS of 1D nanostructures can be expressed as:

$$D(E) = \frac{1}{\pi \hbar v(E)} \quad \text{per spin per valley.}$$

3a) Conduction of (13,0) CNT

Parameters and Settings

Simulate new input parameters

Carbon Nanotube Bands

Learn about Carbon Nanotube physical structure and electronic band structure as you explore the devices in this simulator.

Enter values on the left, then push the Simulate button. Simulation results will appear here.

This application is powered by:
Octave and Fortran 77. Last updated August 30, 2005.

Chirality (n,m)

n: 13

m: 0

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

Length of nanotube in 3-D view: 15

Refresh Screen | Copy/Paste with Desktop

3a) Conduction of (13,0) CNT

Energy Band Structure

Simulate

Result: Output Log

Length of unit cell (na)
0.42600

Number of hexagons (unit cell)
26

DOS Energy Range (eV) [-x : x]
3.0100

Boundary of Brillouin Zone (ktaax)
7.3746e+09

Bandgap Magnitude (eV)
0.81678

Bandgap Magnitude in units of overlap parameter (t)
0.27226

kt at bandgap
3.9220e-19

Chirality (n,m)

n: 13

m: 0

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

Length of nanotube in 3-D view: 15

Find: [] [] []

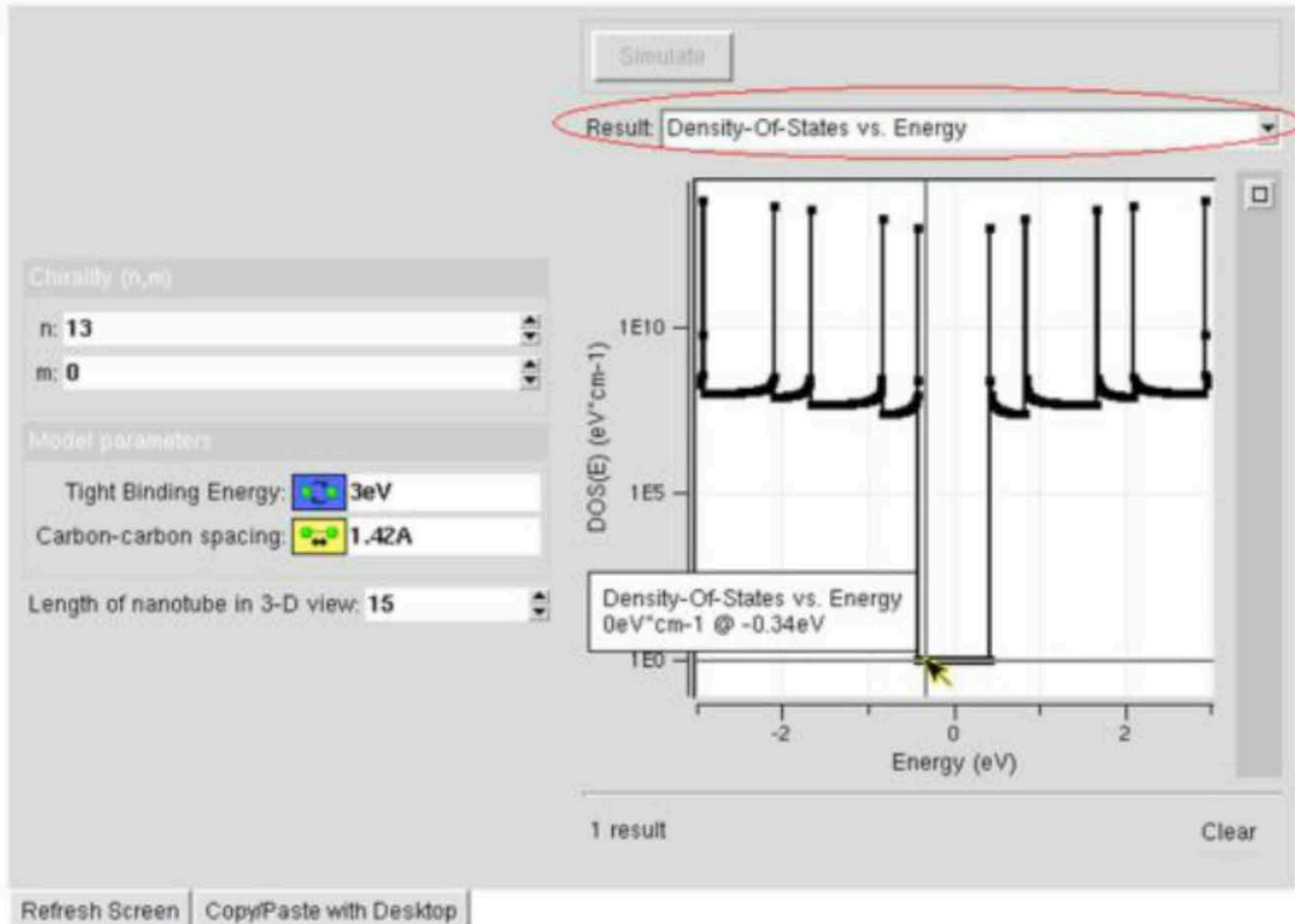
Select All

1 result Clear

Refresh Screen | Copy/Paste with Desktop

3b) DOS of (13,0) CNT

Density of States

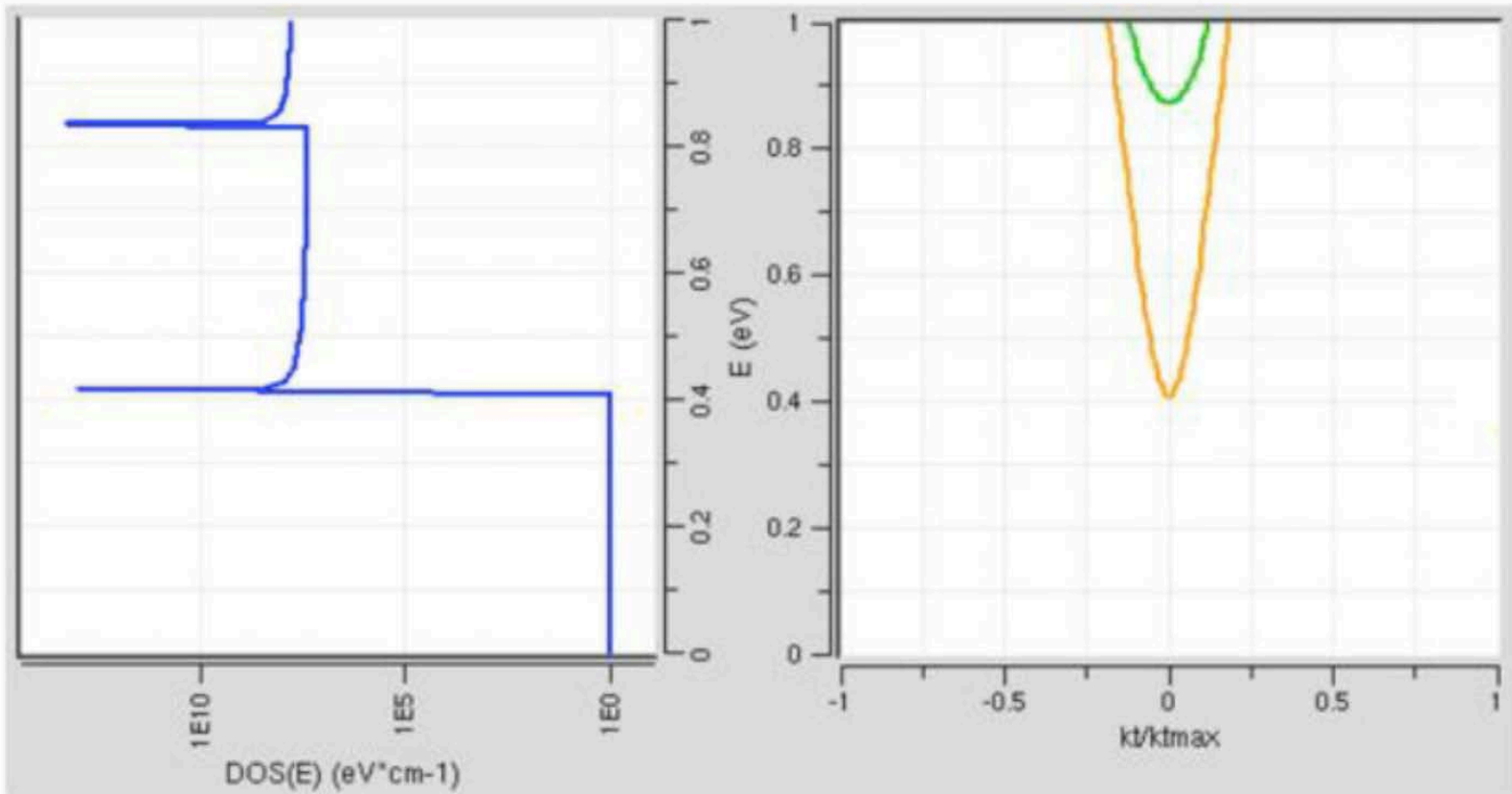


3b) DOS of (13,0) CNT

Singularities in the Density of States

$$D(E) = \frac{1}{\pi \hbar v(E)}$$

$$v(E) = \frac{1}{\hbar} \cdot \frac{dE}{dk}$$



Exercise 4 – Diameter Dependence of CNTs

Simulate $(n, 0)$ zigzag CNTs for $n=12$ to $n=26$

- (a) What percentage of CNTs is metallic, and what percentage is semiconducting?
- (b) Read Mintmire and White, “Universal Density of States for Carbon Nanotubes,” *Phys. Rev. Lett.*, 81, 2506, 1998. State the condition for a CNT to be metallic and the condition for a CNT to be semiconducting.
- (c) For semiconducting CNTs, plot the bandgap as a function of the CNT diameter
- (d) Can the plot be fitted by $E_g = E_0 / d$ (in nm) where d is the CNT diameter? If so, what is the fitting value E_0 ?

4a) & 4b) Metallic and Semiconducting CNTs

4a)

Reference:

Lundstrom M., Guo J. “Nanoscale Transistors Device Physics, Modeling and Simulation,” 2006 Springer Science+Business Media Inc. New York, NY p. 164

33% of CNTs are metallic

67% of CNTs are semiconducting

4b)

Chirality of CNT described by (n_1, n_2)

Metallic if $(n_1 - n_2)$ is an integer multiple of 3

Semiconducting otherwise

4c) Bandgap Versus Diameter: Plot

Obtaining Data Points

The screenshot shows a simulation interface with the following parameters and results:

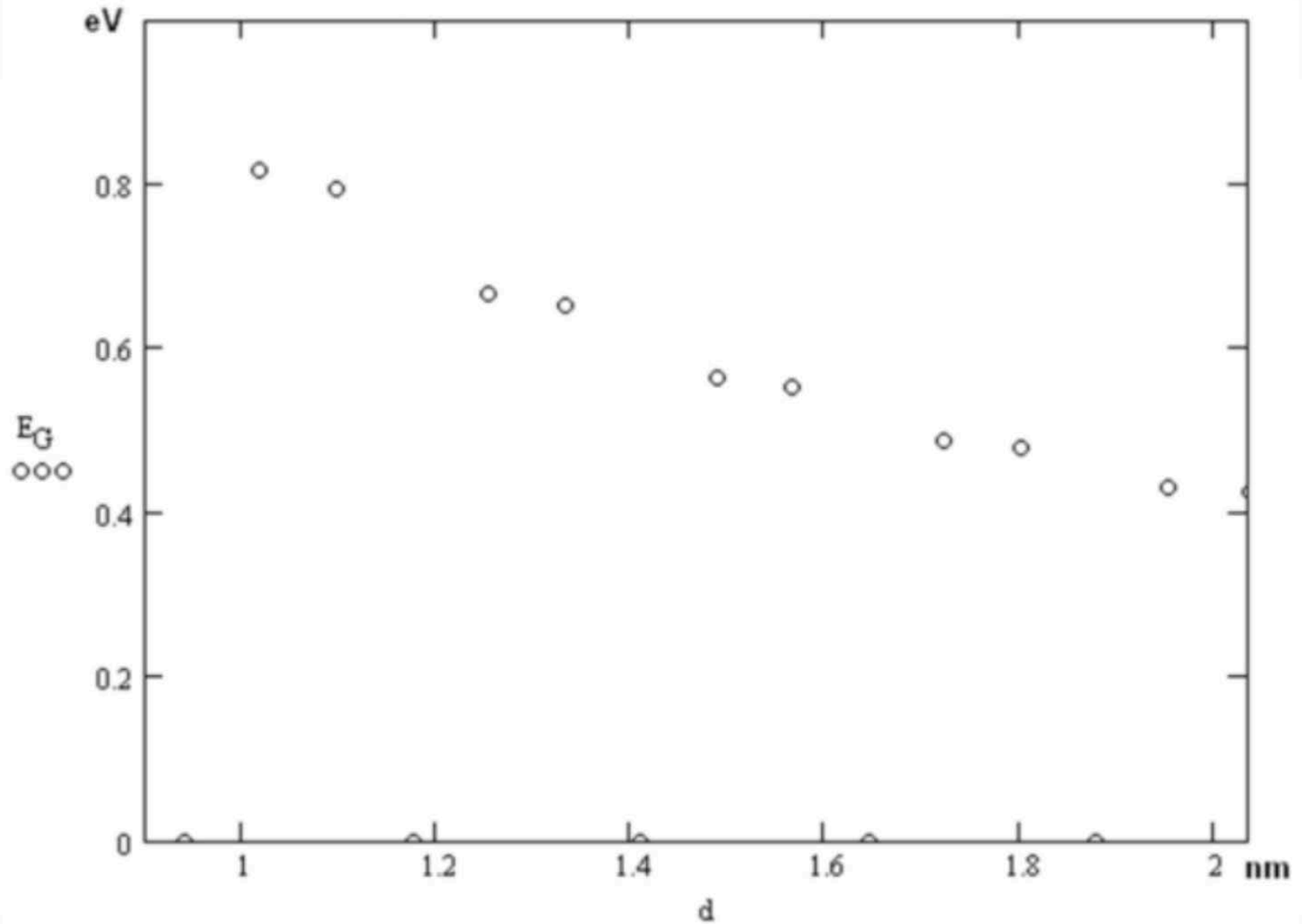
Chirality (n,m)
n: 12
m: 0

Model parameters
Tight Binding Energy: 3eV
Carbon-carbon spacing: 1.42A
Length of nanotube in 3-D view: 15

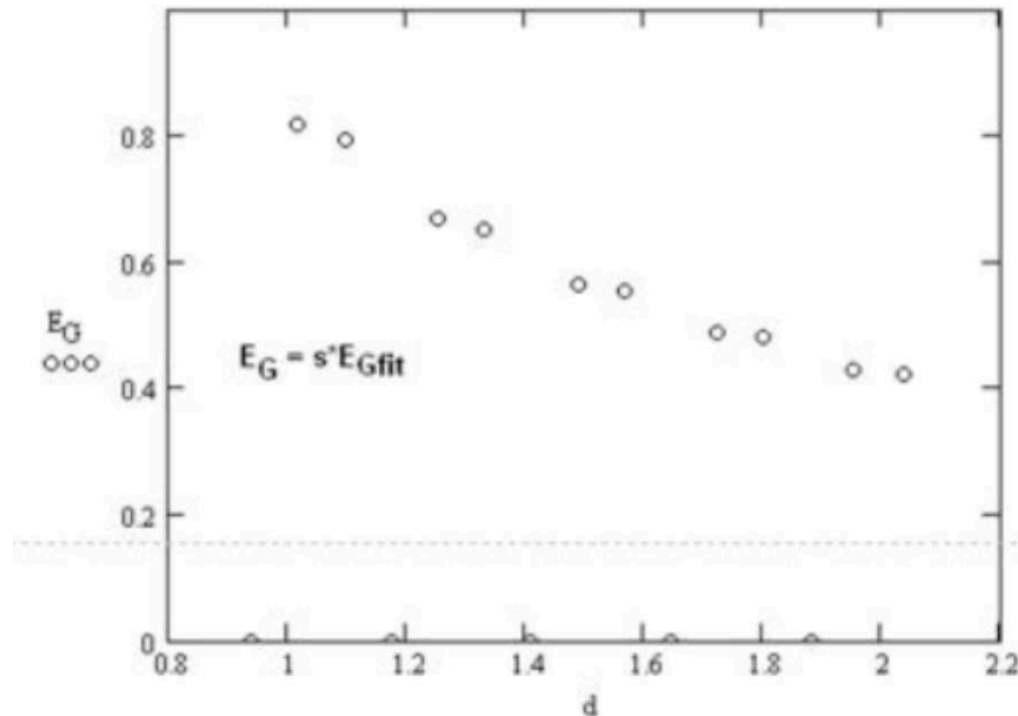
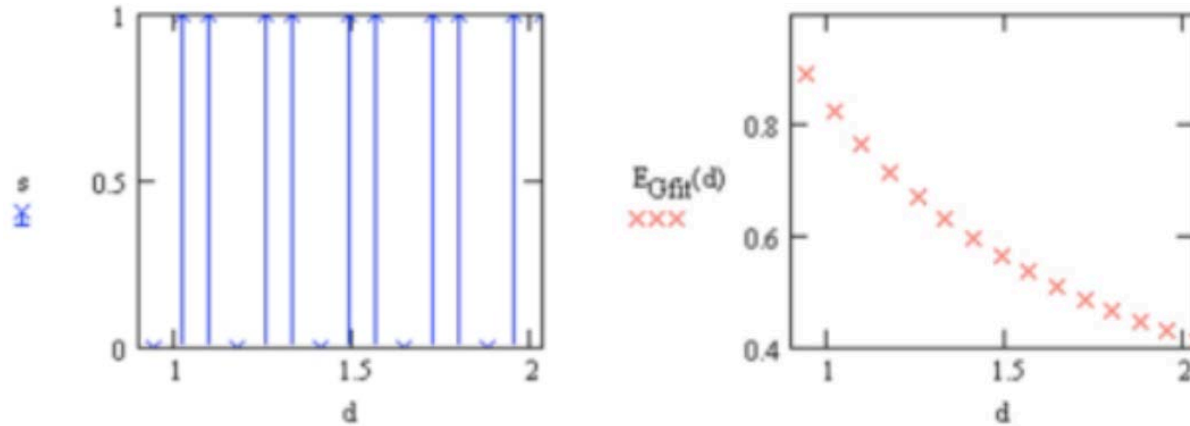
Results:
Length of unit cell (nm): 0.42600
Number of hexagons (unit cell): 24
DOS Energy Range (eV) [-x : x]: 3.0100
Boundary of Brillouin Zone (ktmax): 7.3746e+09
Bandgap Magnitude (eV): 0
Bandgap Magnitude in units of overlap parameter (t): 0
kt at bandgap: -4.0412e-17

Buttons: Simulate, Find, Select All, Clear, Refresh Screen, Copy/Paste with Desktop

4b) Bandgap Versus Diameter: Plot



4d) Bandgap Versus Diameter: Fit



4d) Bandgap Versus Diameter: Fit

Constant resulting from $n = 19$: $E_0 = .838\text{eVnm}$

