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?

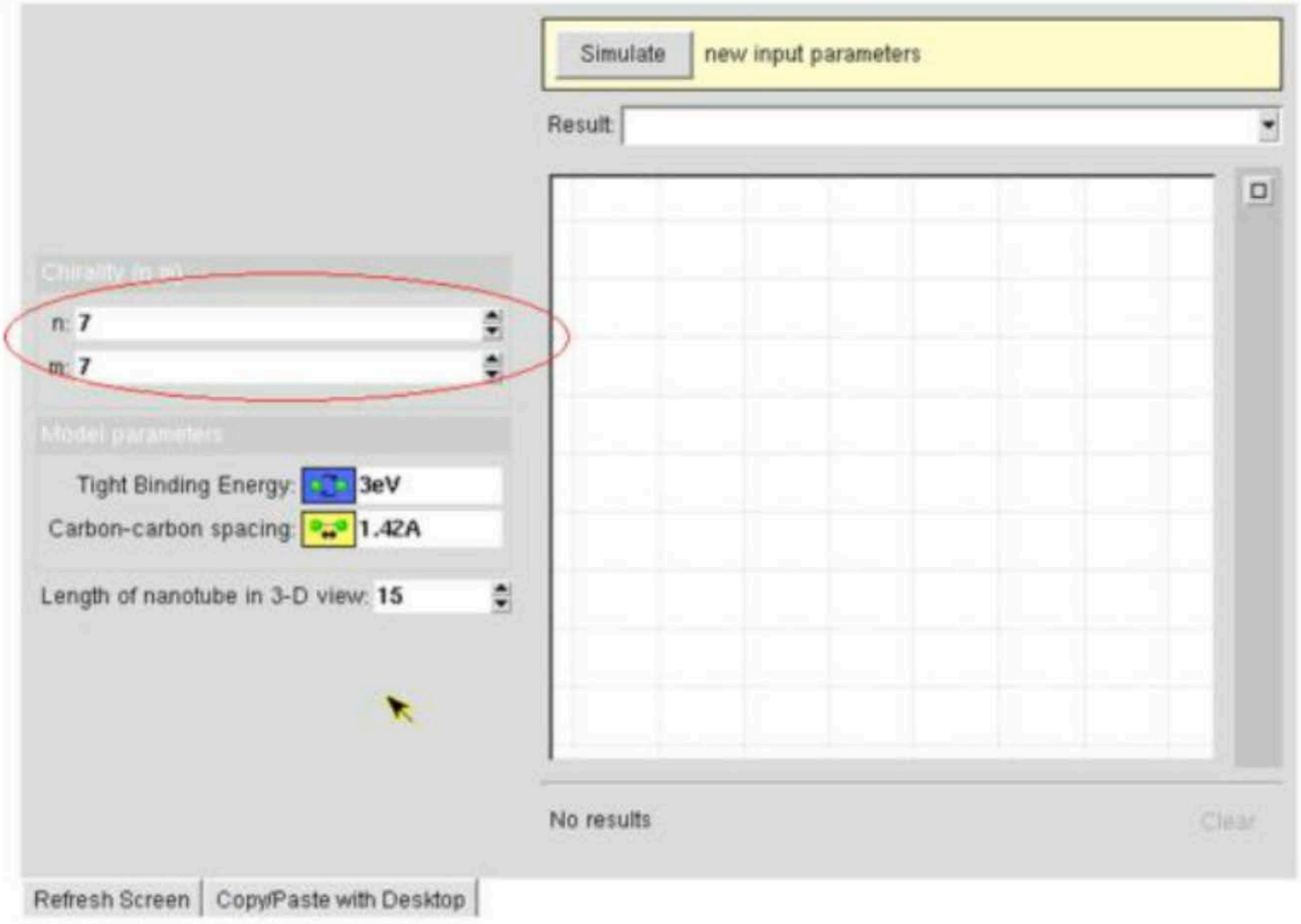
(b) simulate a (13,0) CNT and print out its unit cell structure. Why are CNTs with n=0 called zigzag CNTs? What is the length of a unit cell?

(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?

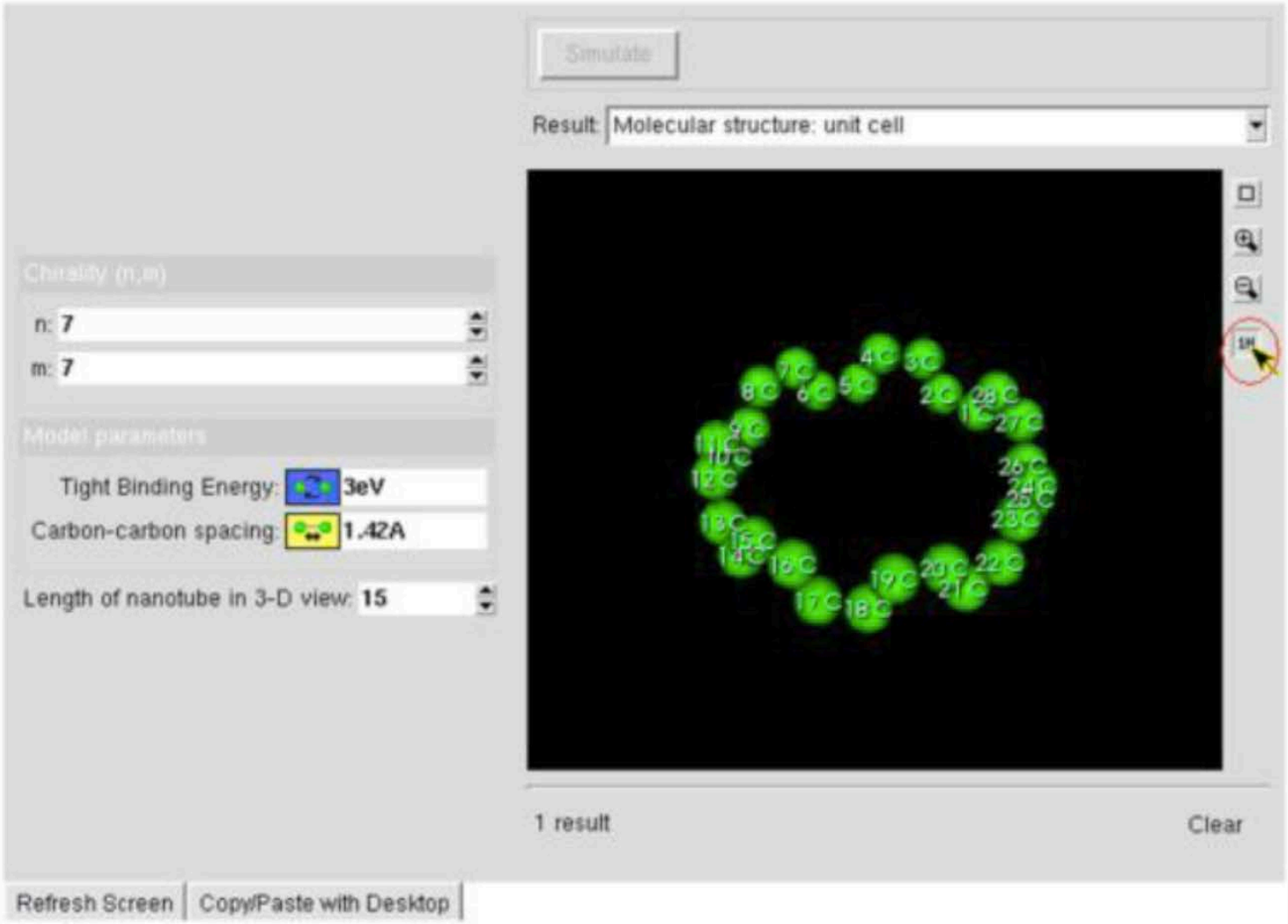
1a) (7,7) CNT

Parameters and Settings



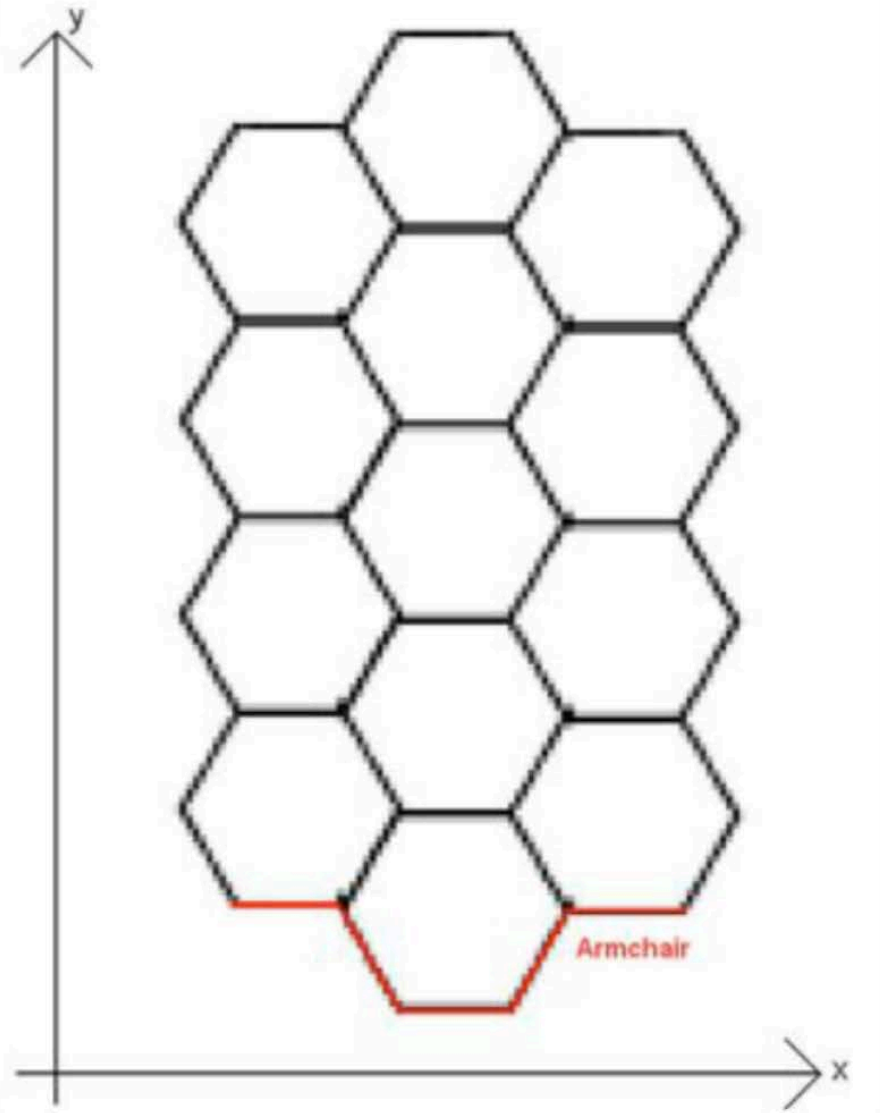
1a) (7,7) CNT

Unit Cell Structure



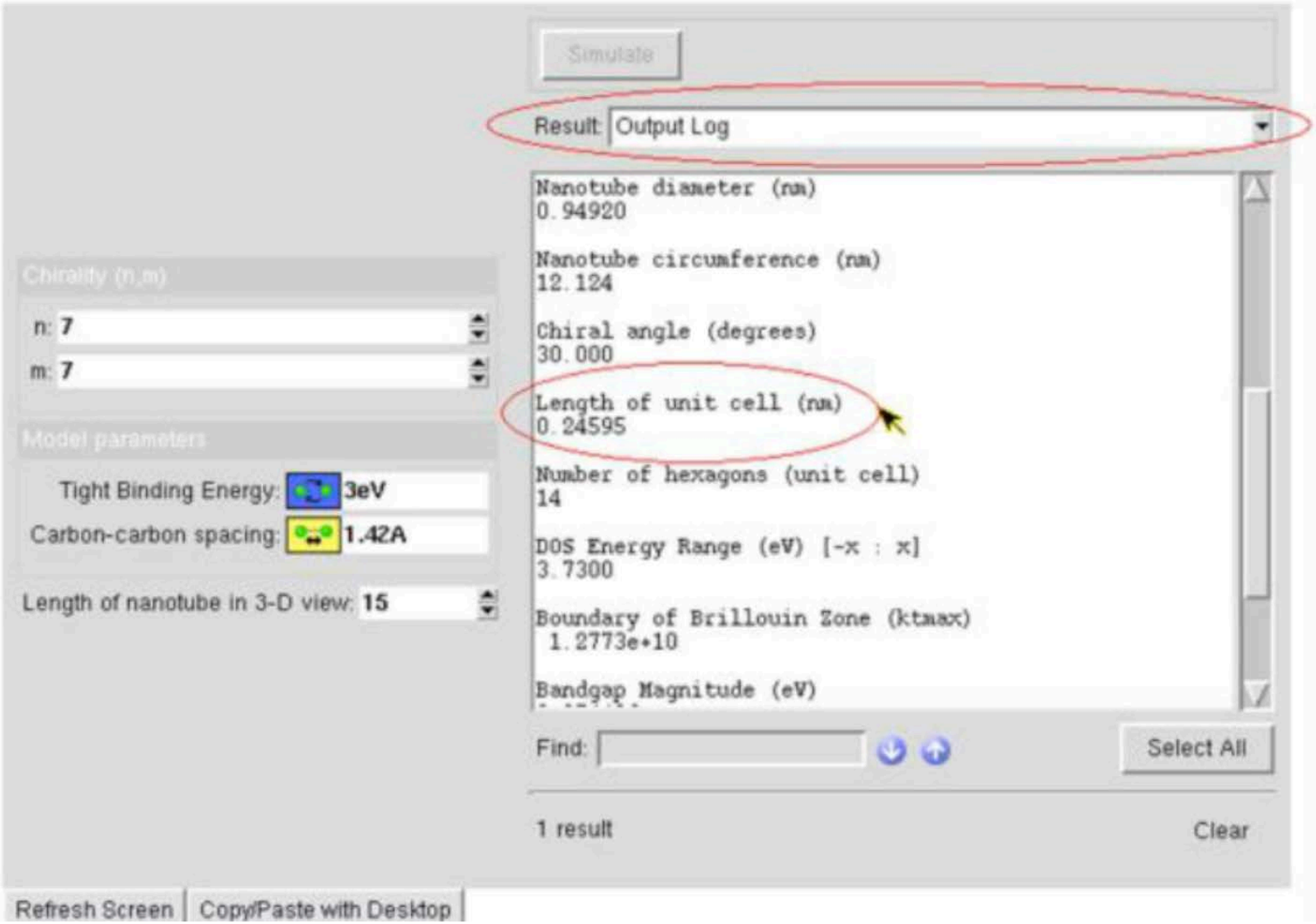
1a) (7,7) CNT

Nomenclature: Armchair

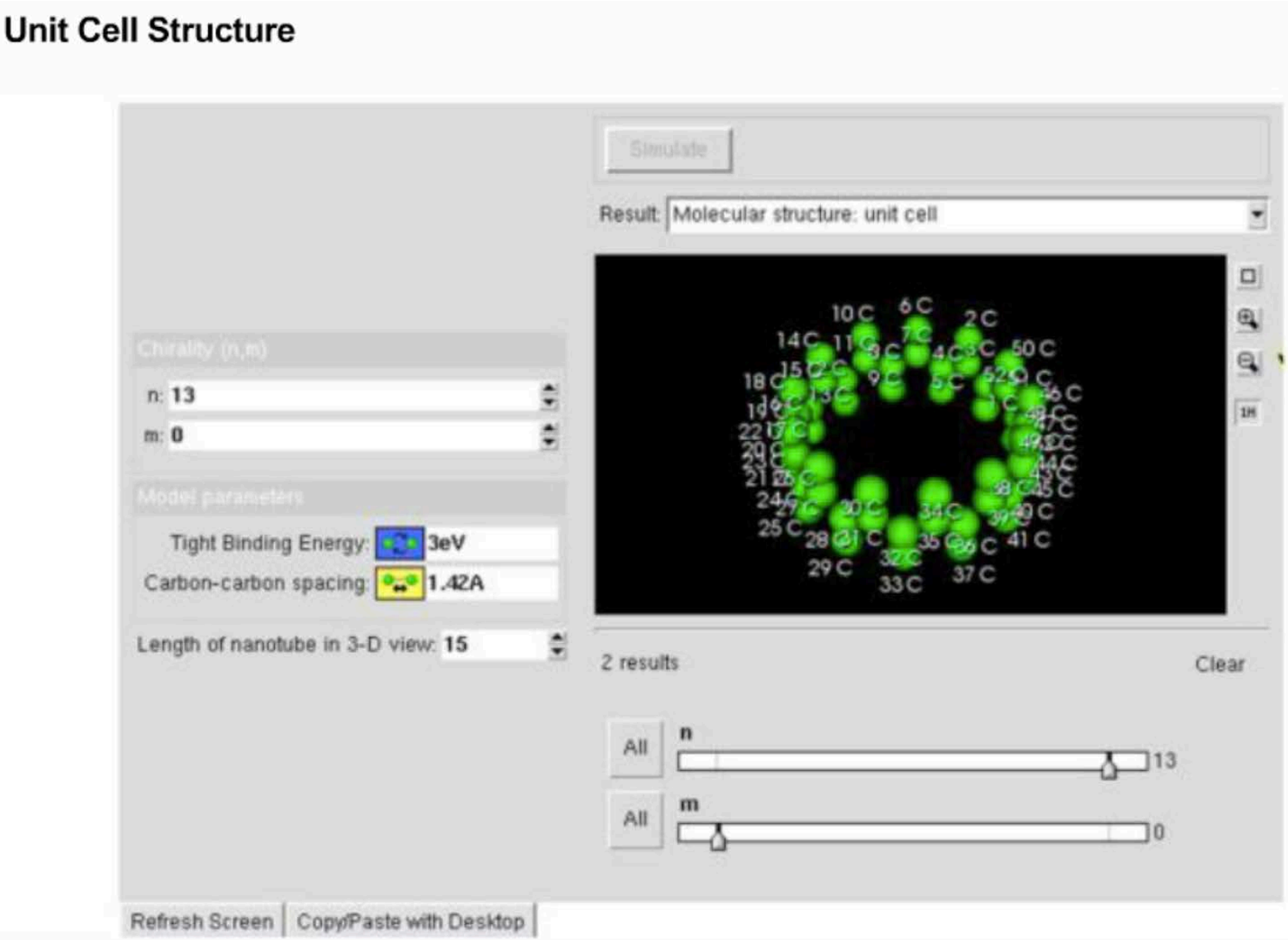


1a) (7,7) CNT

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

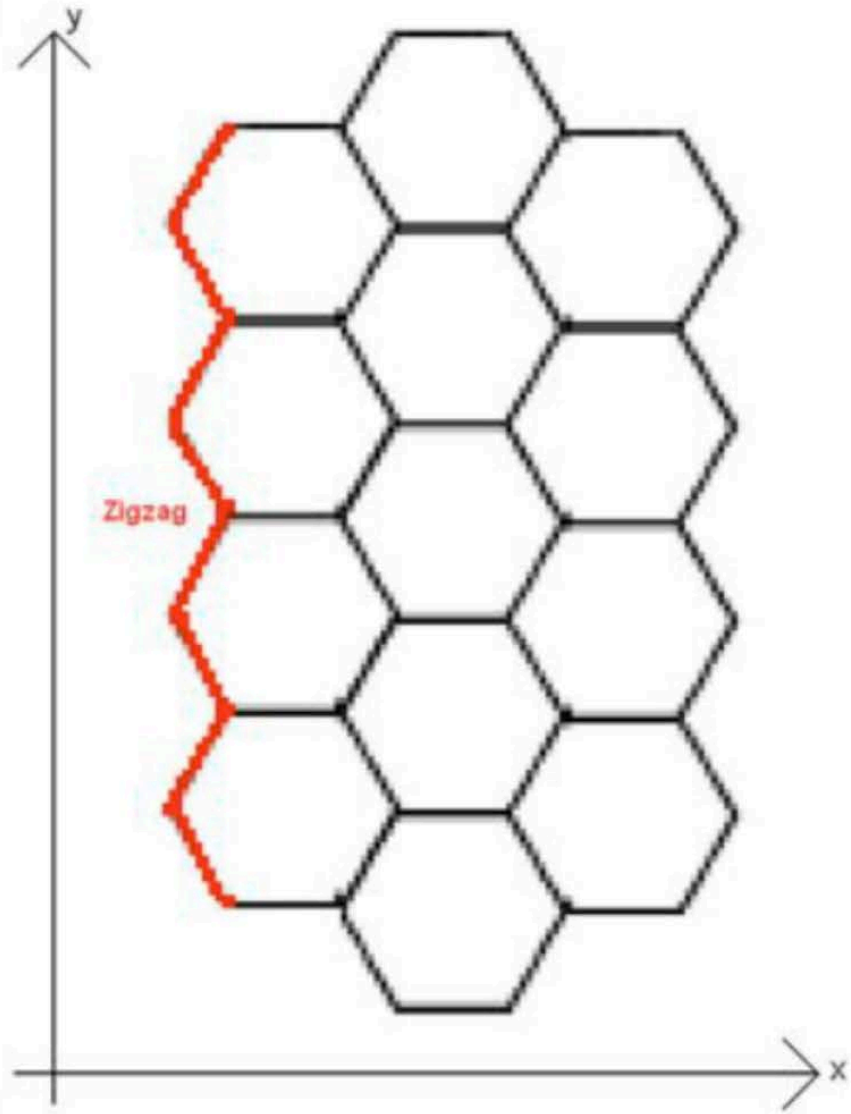


1b) (13,0) CNT


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: 1.42A
Length of nanotube in 3-D view: 15
2 results
Clear
All
n
13
All
m
0
Refresh Screen
Copy/Paste with Desktop

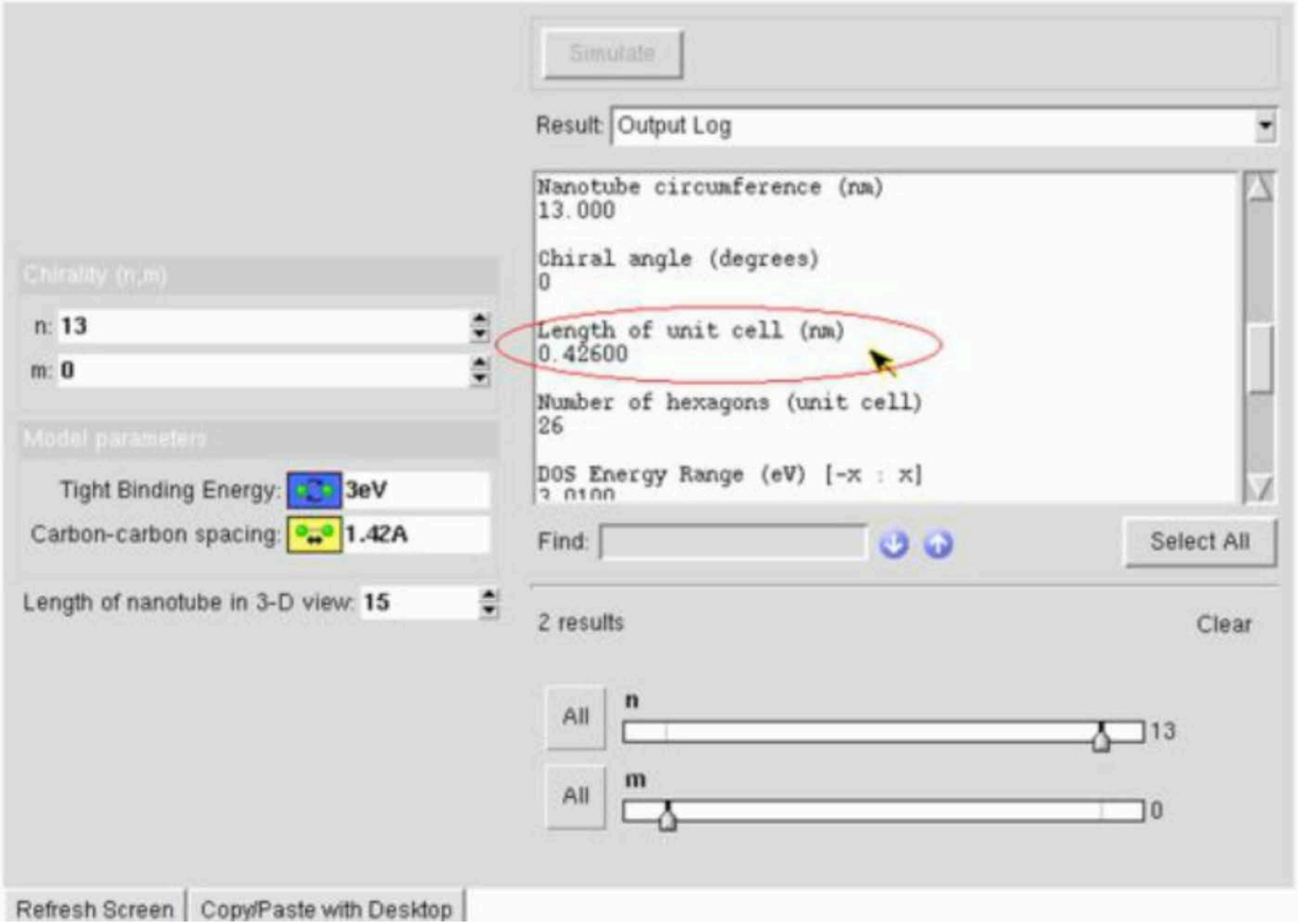
1b) (13,0) CNT

Nomenclature: Zigzag

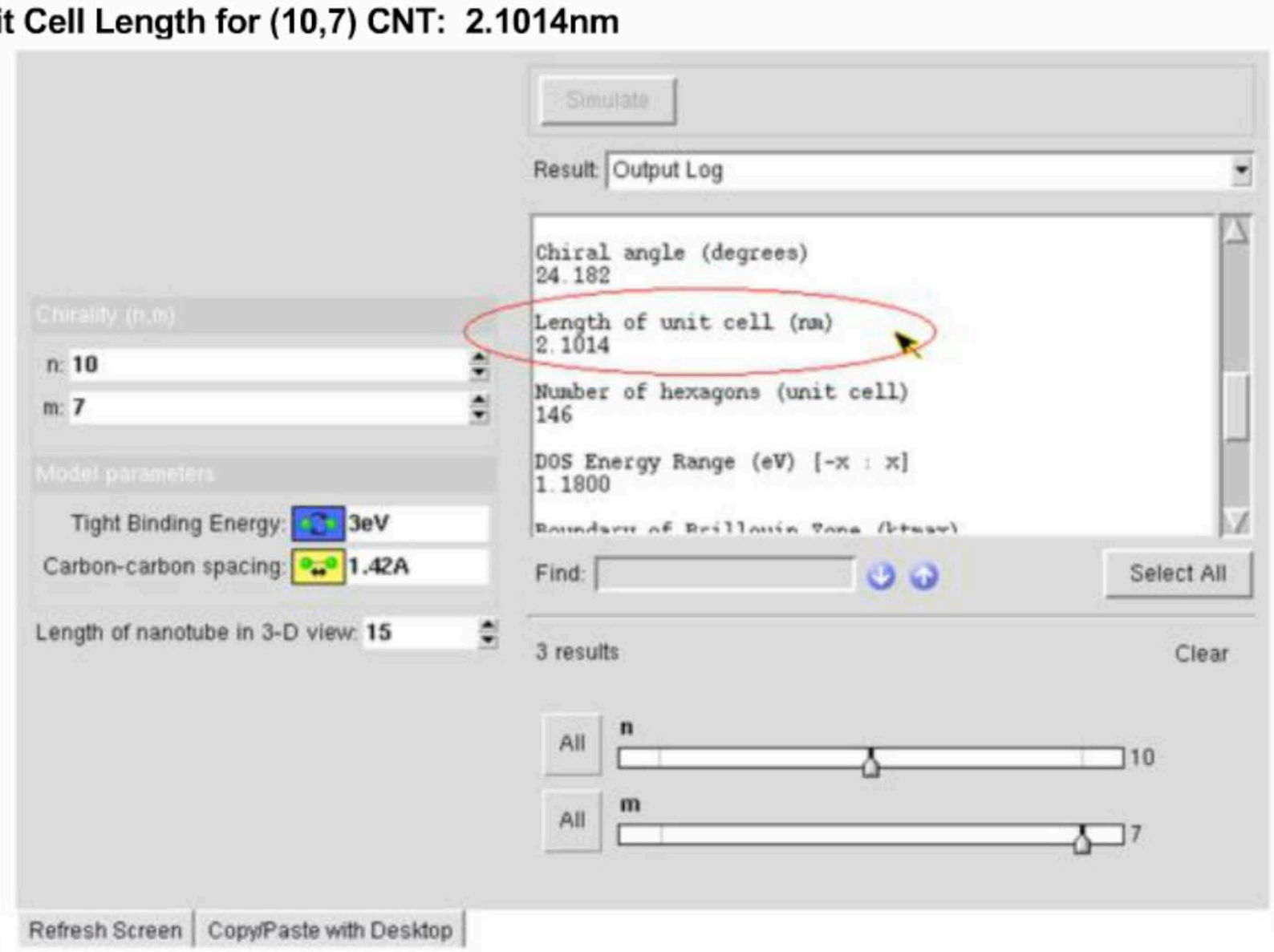


1b) (13,0) CNT

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



1c) (10,7) CNT


Unit Cell Length for (10,7) CNT: 2.1014nm
Simulate
Result: Output Log
Chiral angle (degrees)
24.182
Length of unit cell (nm)
2.1014
Number of hexagons (unit cell)
146
DOS Energy Range (eV) [-x : x]
1.1800
Chirality (n,m)
n: 10
m: 7
Model parameters
Tight Binding Energy: 3eV
Carbon-carbon spacing: 1.42A
Length of nanotube in 3-D view: 15
Find:
Select All
3 results
Clear
All
n
10
All
m
7
Refresh Screen
Copy/Paste with Desktop

1d) Unit Cell Length

The referenced equation is:

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

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

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

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

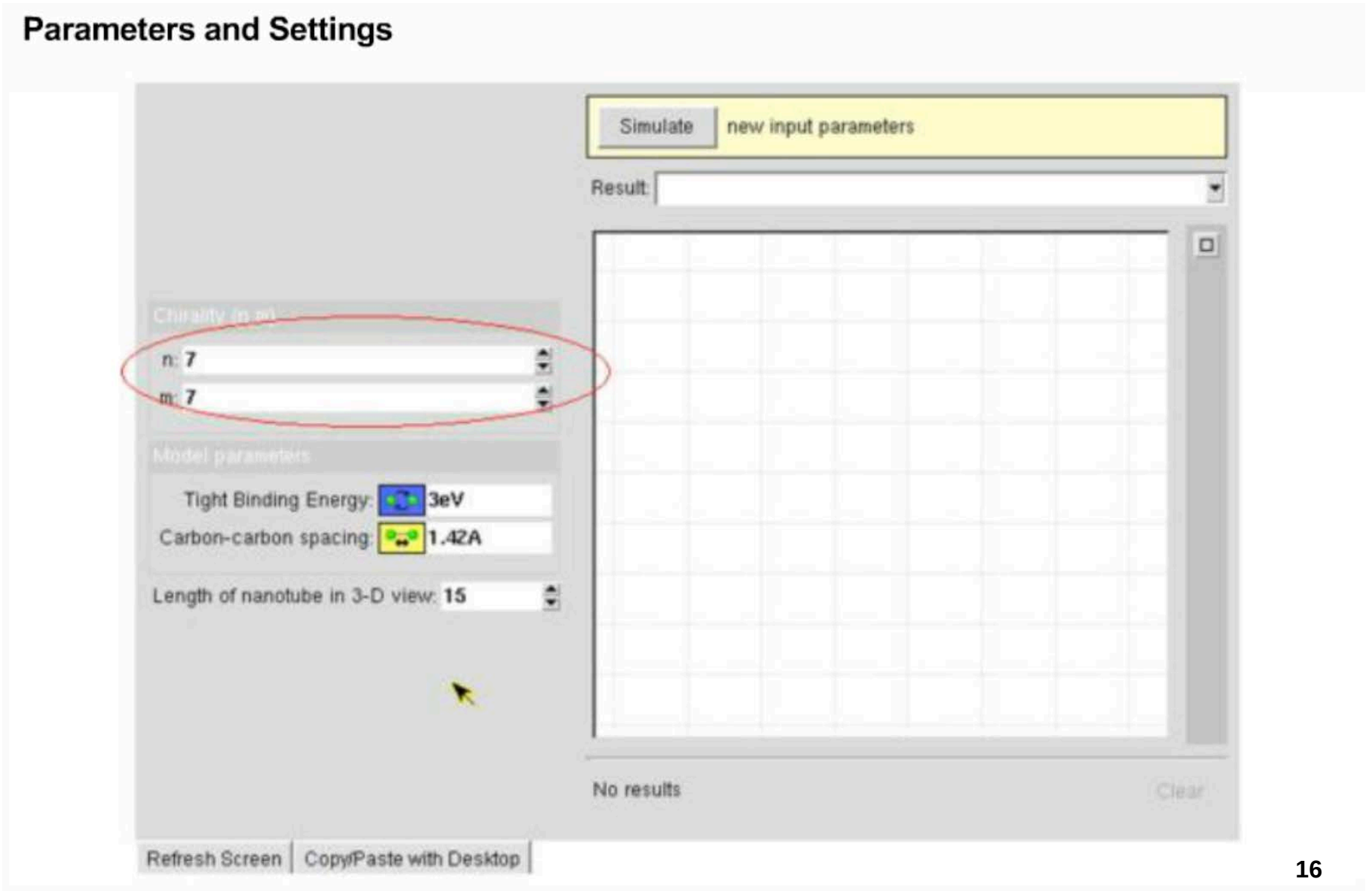
(a) Is the CNT metallic or semiconducting? How many valleys are there in a Brillouin zone?

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

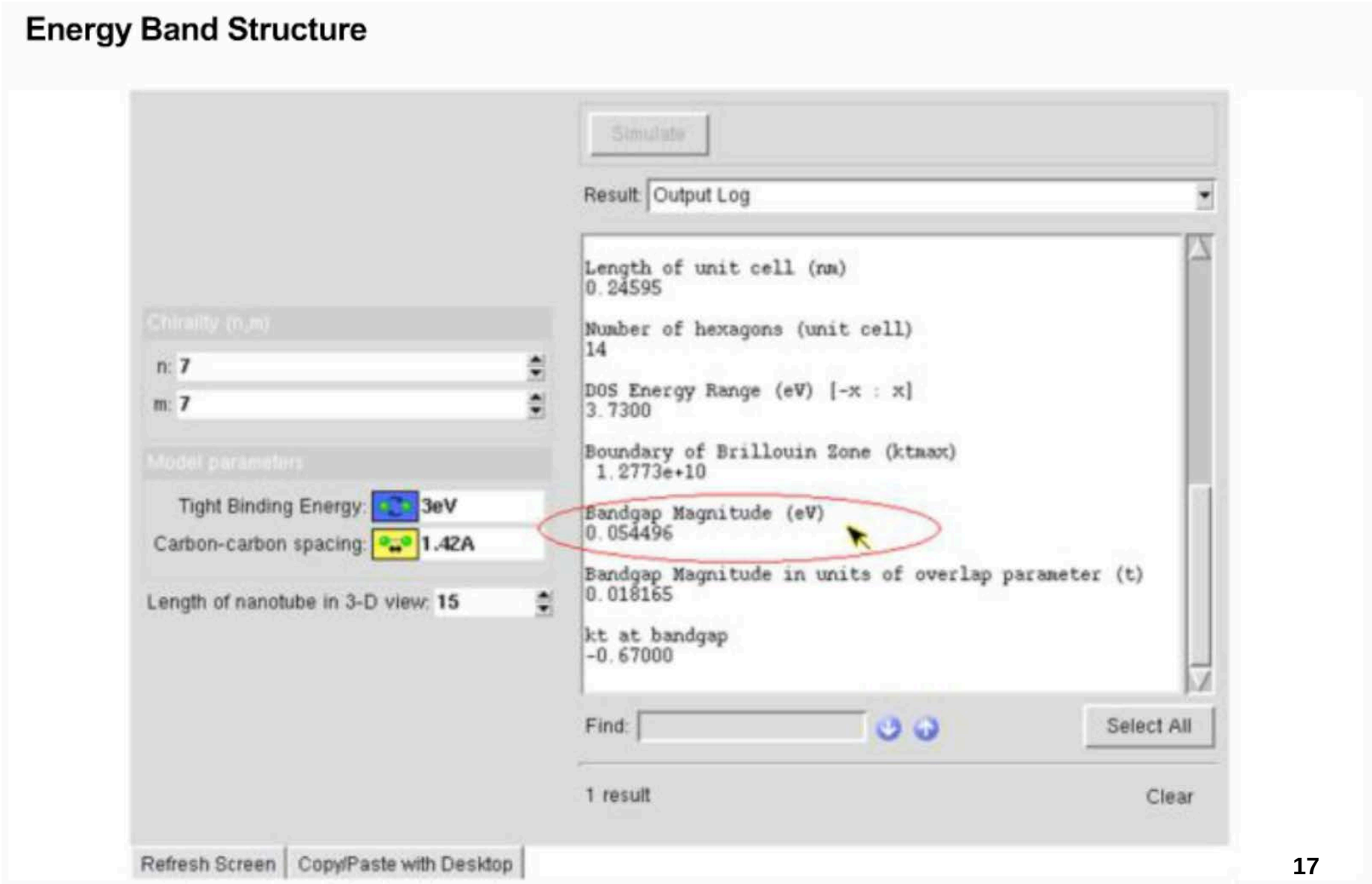
(c) What is the carrier velocity near the Fermi level?

(d) What is the simulated density of states near the Fermi level? How does it compare to the computed value, $D(E) = \frac{4}{\pi \hbar \upsilon_F}$ *?*

2a) Conduction of (7,7) CNT

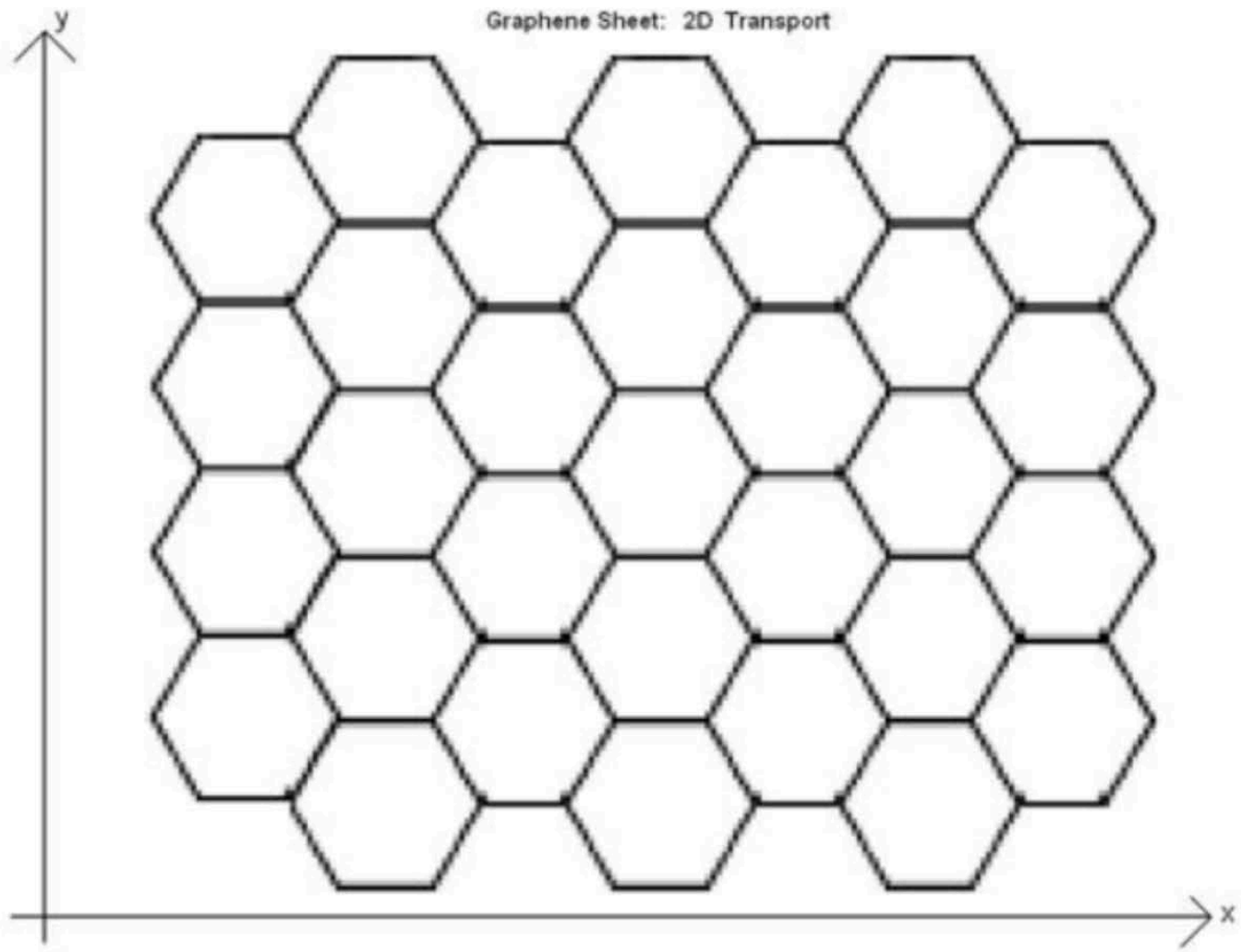


2a) Conduction of (7,7) CNT



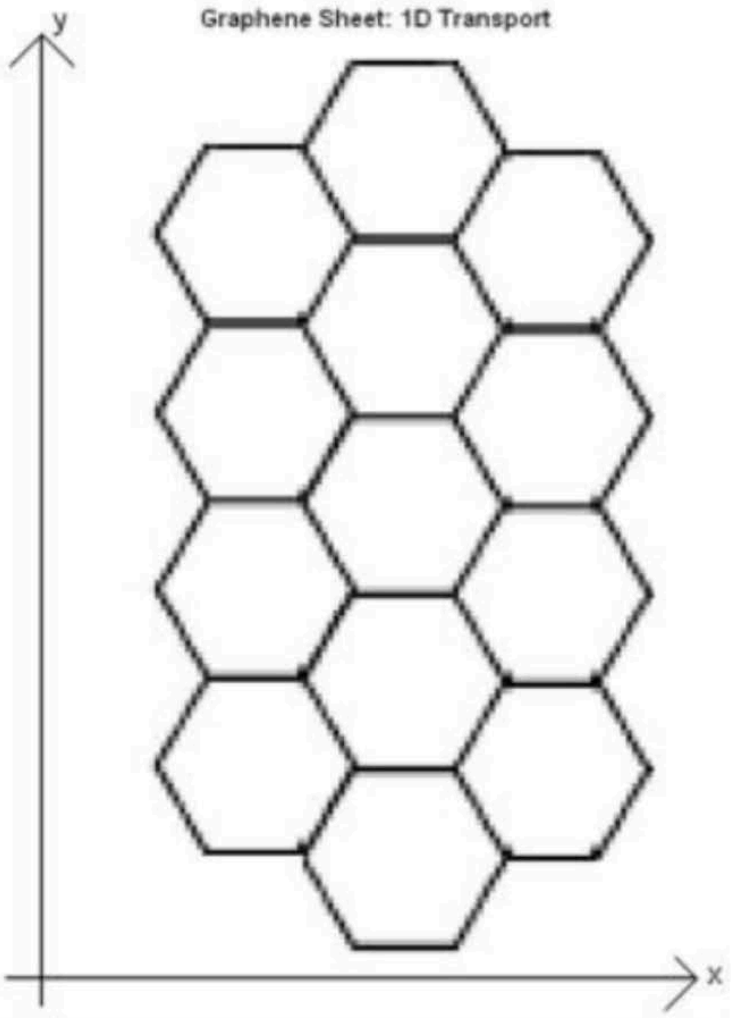
2b) Zone-Folding Method

Zone-Folding Method: Metallic Property of Armchair CNTs



2b) Zone-Folding Method

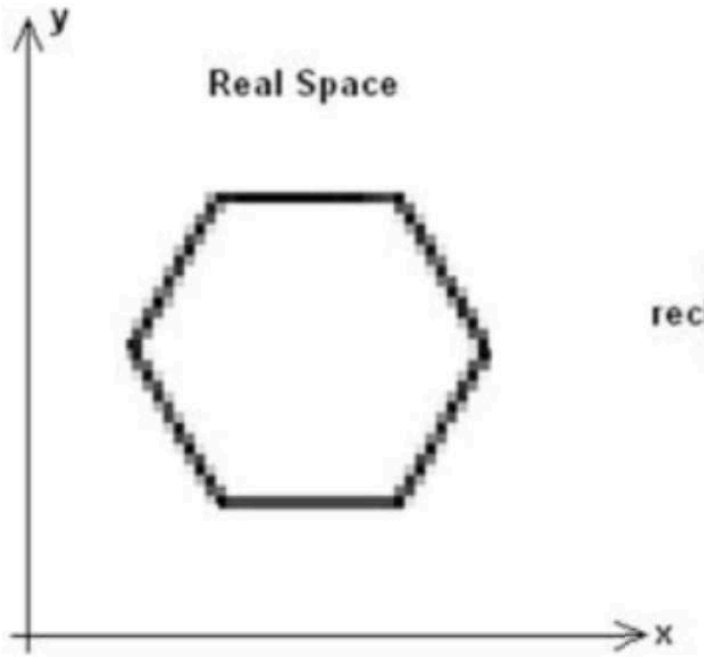
Zone-Folding Method: Metallic Property of Armchair CNTs



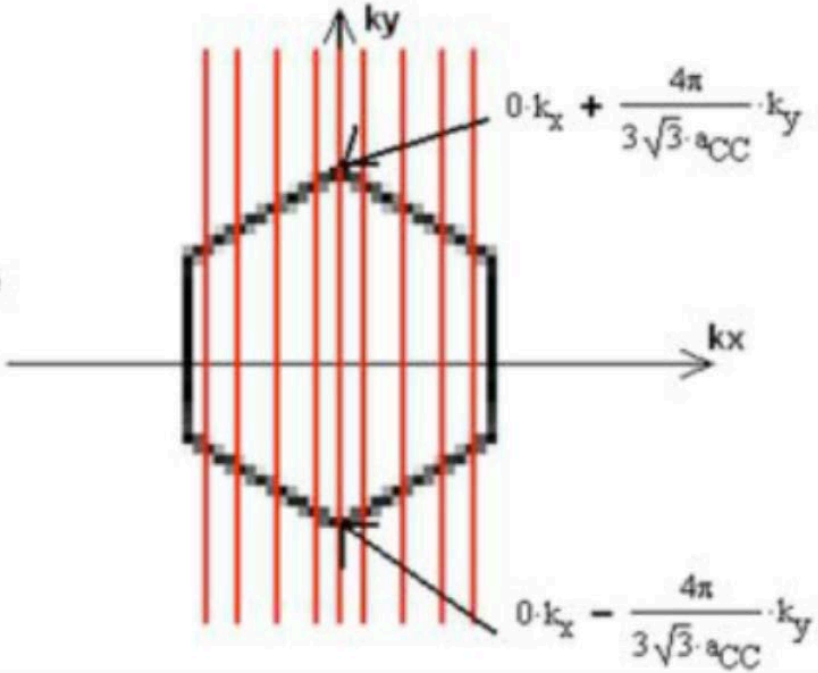
2b) Zone-Folding Method

Zone-Folding Method: Metallic Property of Armchair CNTs

Graphene Fermi Points: $0 \cdot k_x +/- \frac{4\pi}{3 \cdot \sqrt{3}\, a_{CC}} \cdot k_y$



convert to reciprocal space →



2c) Carrier Velocity

Computing v_F:

$$v_F = \frac{1}{h_{bar}} \cdot \frac{dE}{dk}$$

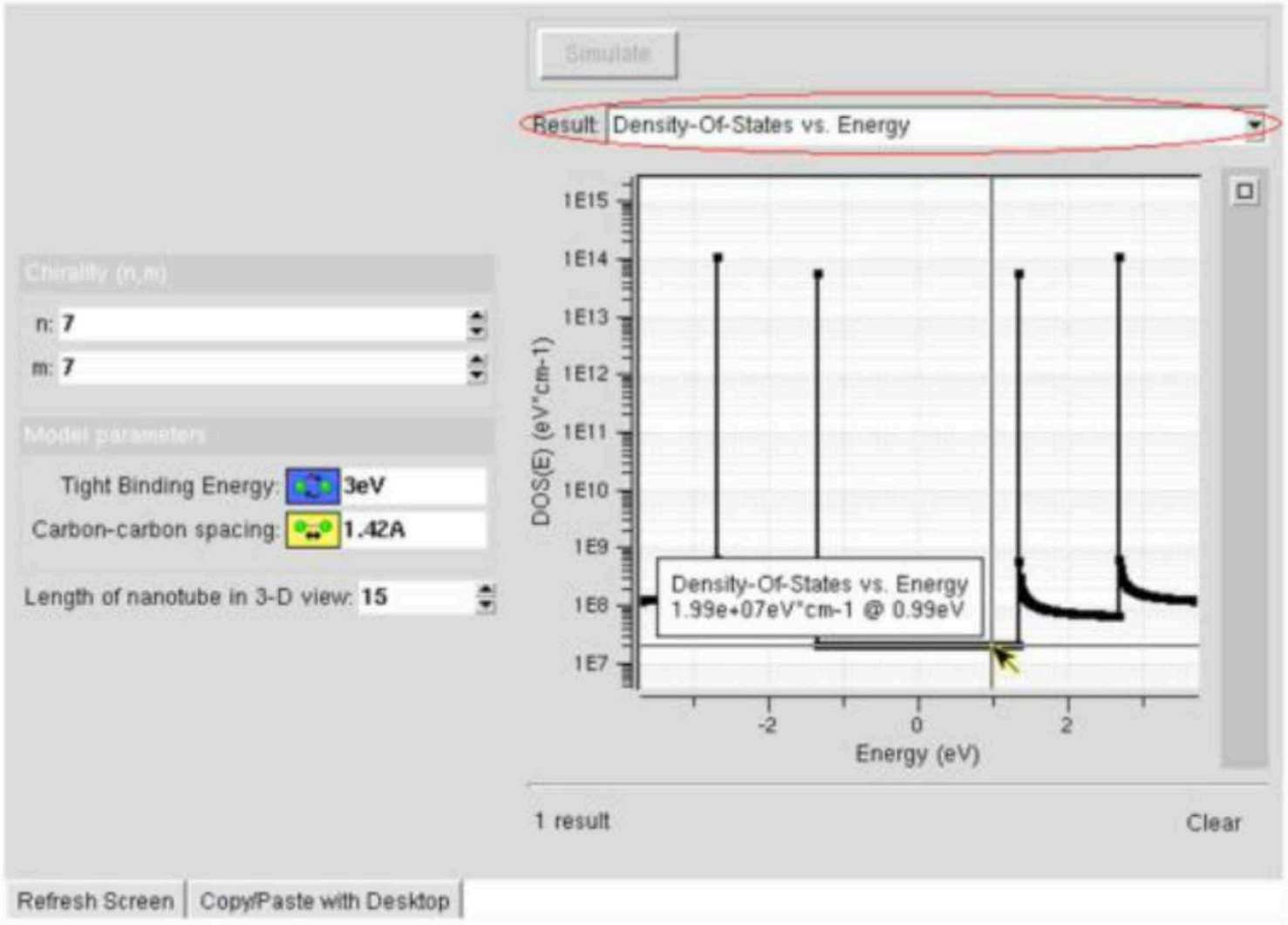
$$k_{tmax} = \frac{\pi}{\sqrt{3} \cdot a_{CC}} \qquad a_{CC} = 1.42\text{Ang}$$

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

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

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

2d) DOS near Fermi Level



2d) DOS near Fermi Level

DOS at Fermi Level Simulation Result: 1.99E7/eVcm

Computed Value:

$$D(E) = \frac{4}{\pi h_{bar} \cdot v_F}$$

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

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

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?

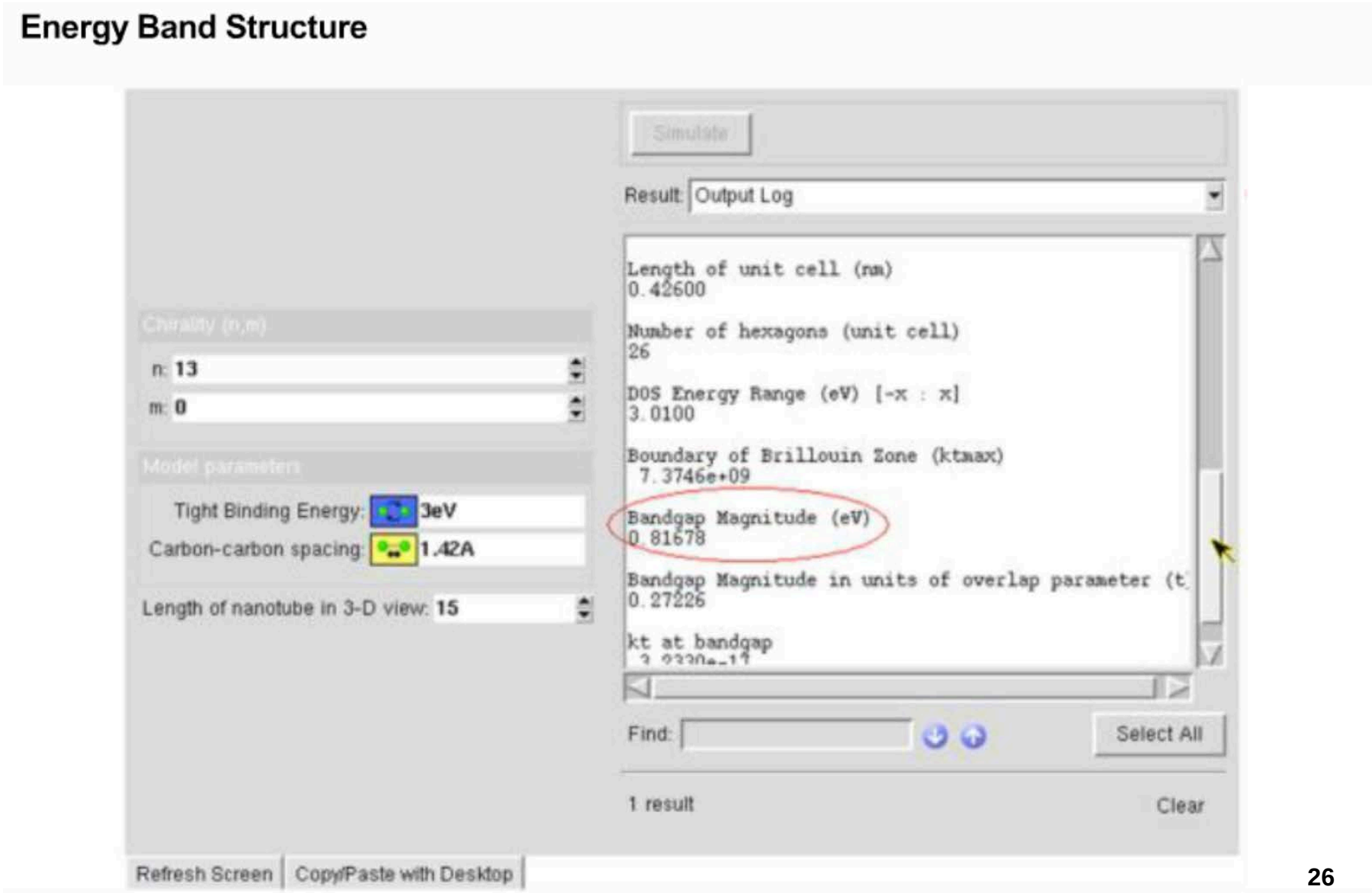
(b)Plot the density-of-states, why does it show singularities at the subband gaps?

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

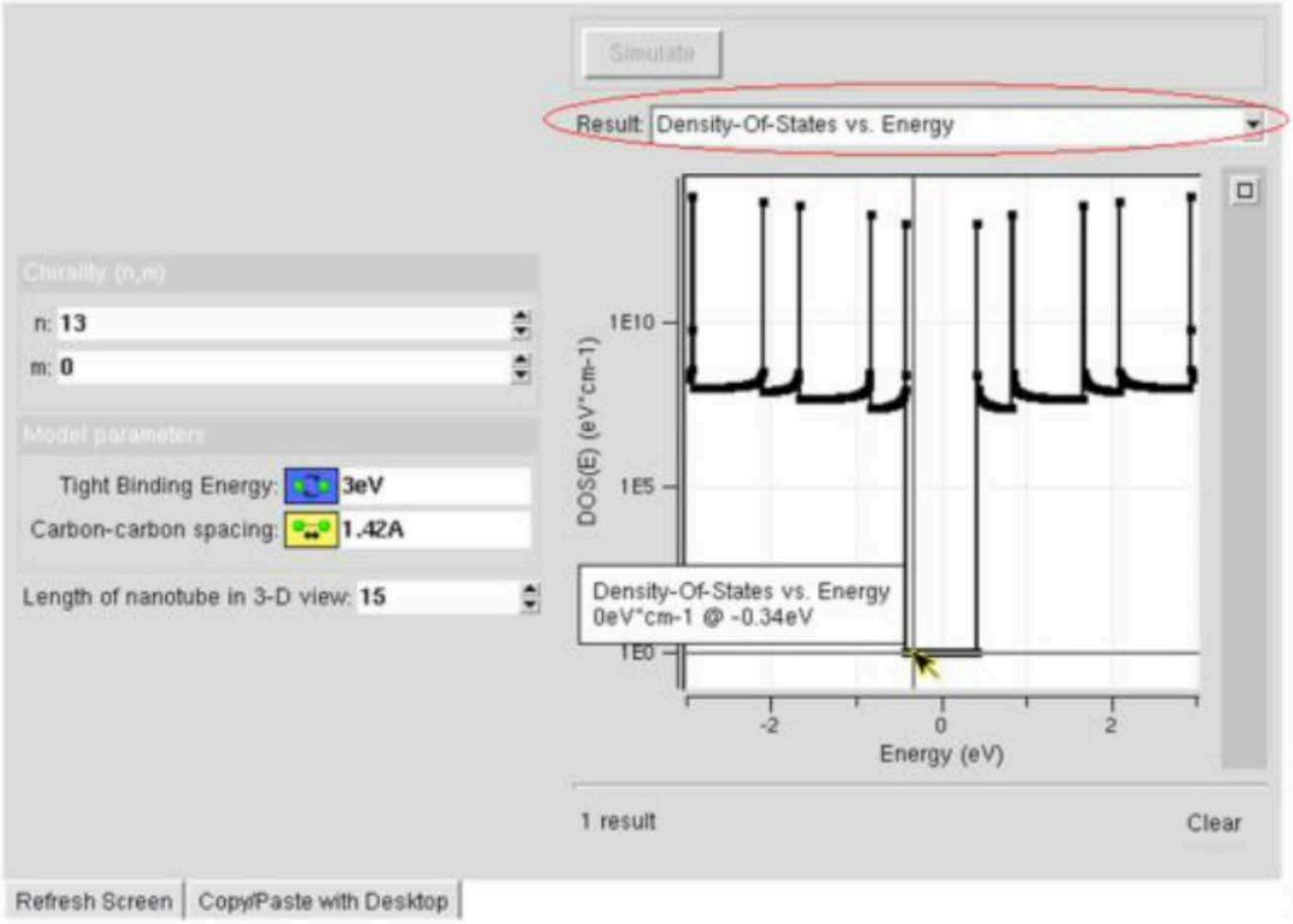
$$D(E)=\frac{1}{\pi\hbar\upsilon(E)}$$ *per spin per valley.*

3a) Conduction of (13,0) CNT

3a) Conduction of (13,0) CNT



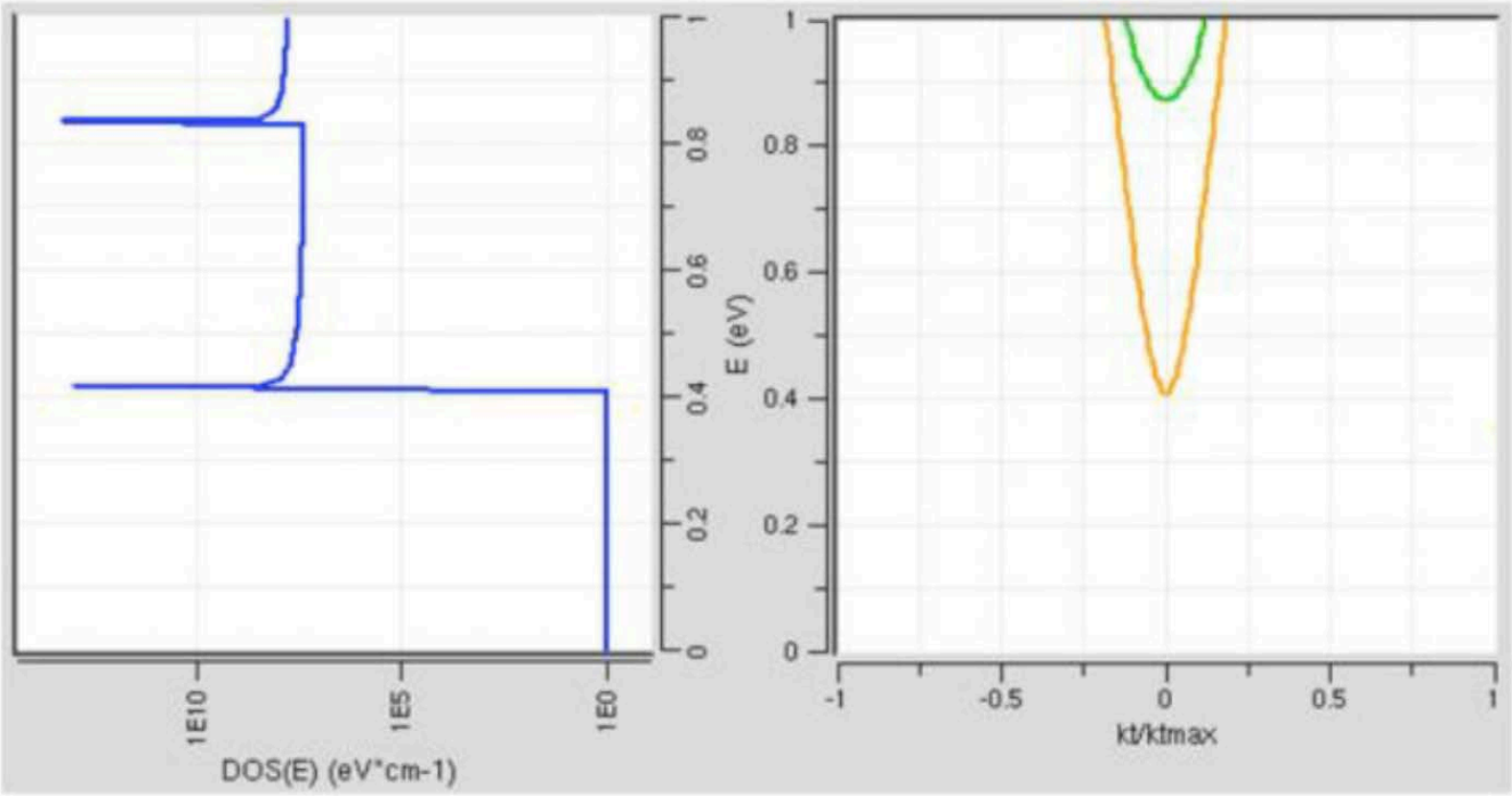
3b) DOS of (13,0) CNT



3b) DOS of (13,0) CNT

Singularities in the Density of States

$$D(E) = \frac{1}{\pi \hbar \upsilon(E)} \qquad \nu(E) = \frac{1}{h_{bar}} \cdot \frac{dE}{dk}$$



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 , $E_g = E_0 / d\,(\text{in nm})$ *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)

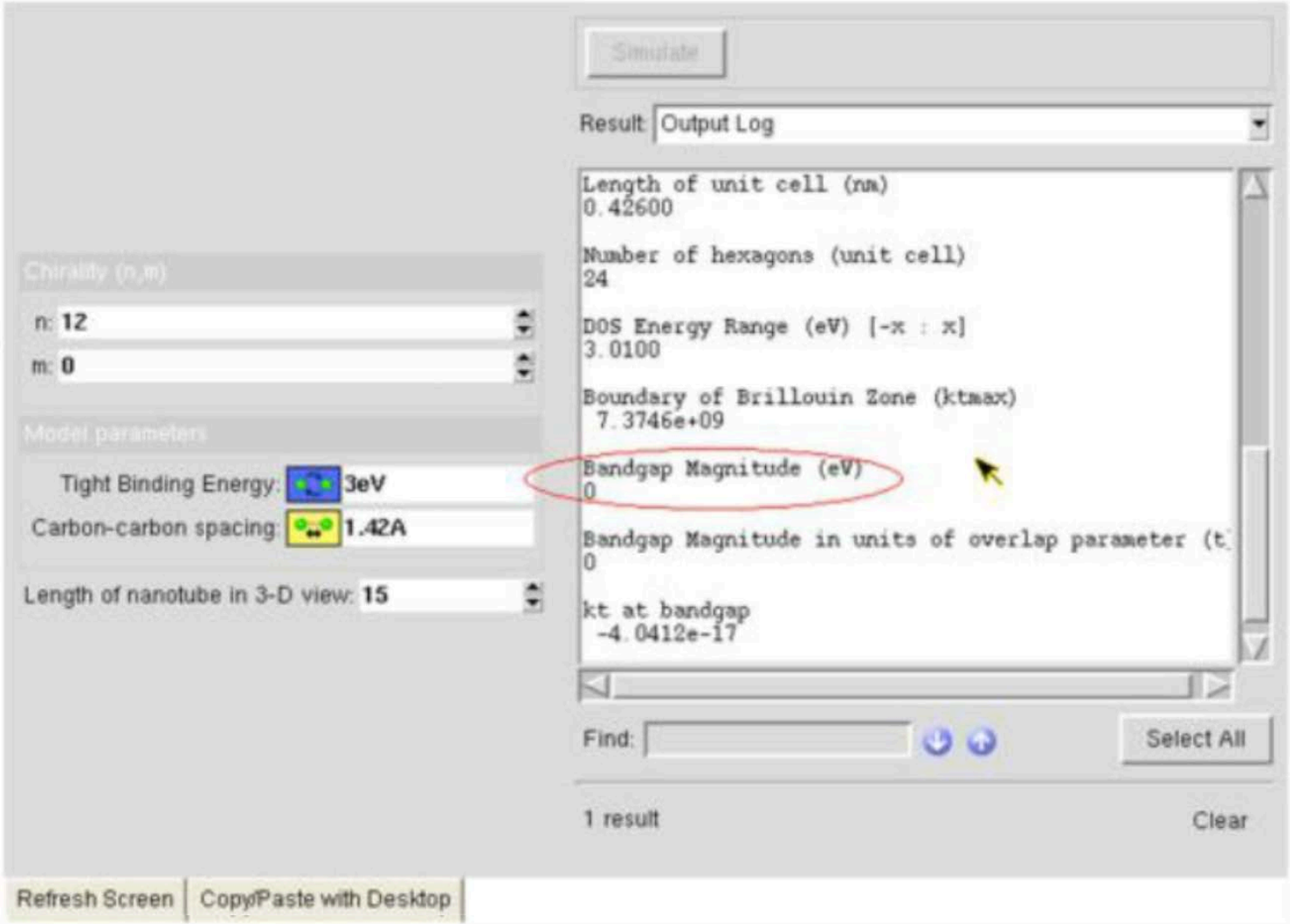
Chirality of CNT described by (n_1,n_2)

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

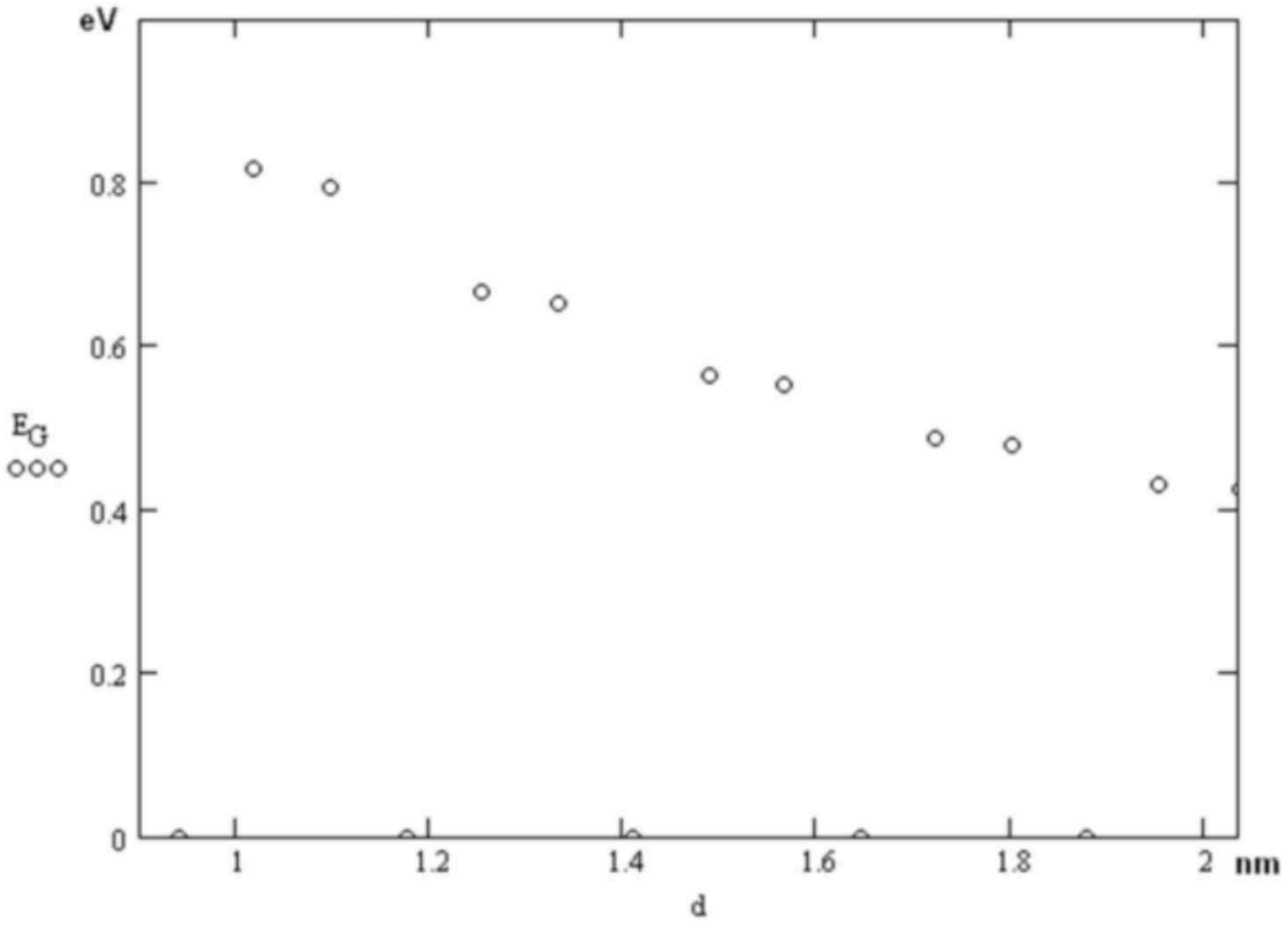
Semiconducting otherwise

4c) Bandgap Versus Diameter: Plot

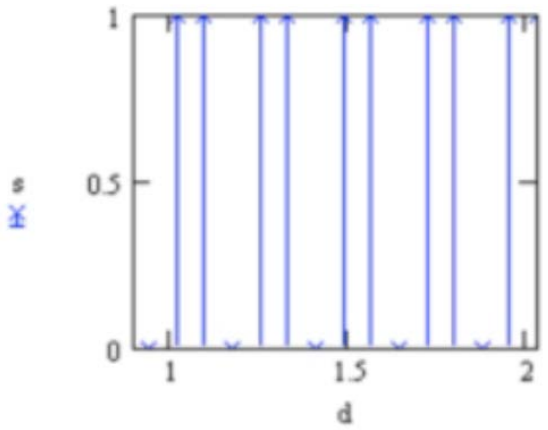
Obtaining Data Points

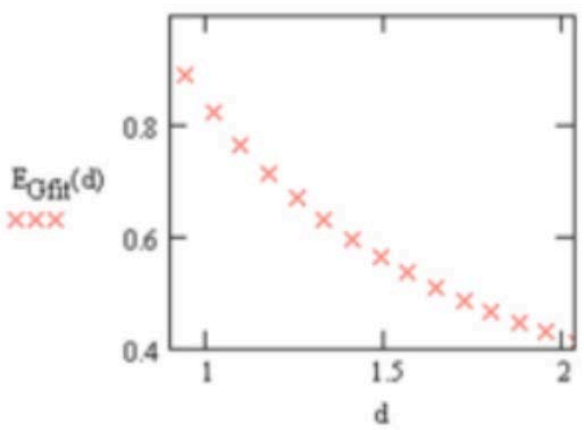


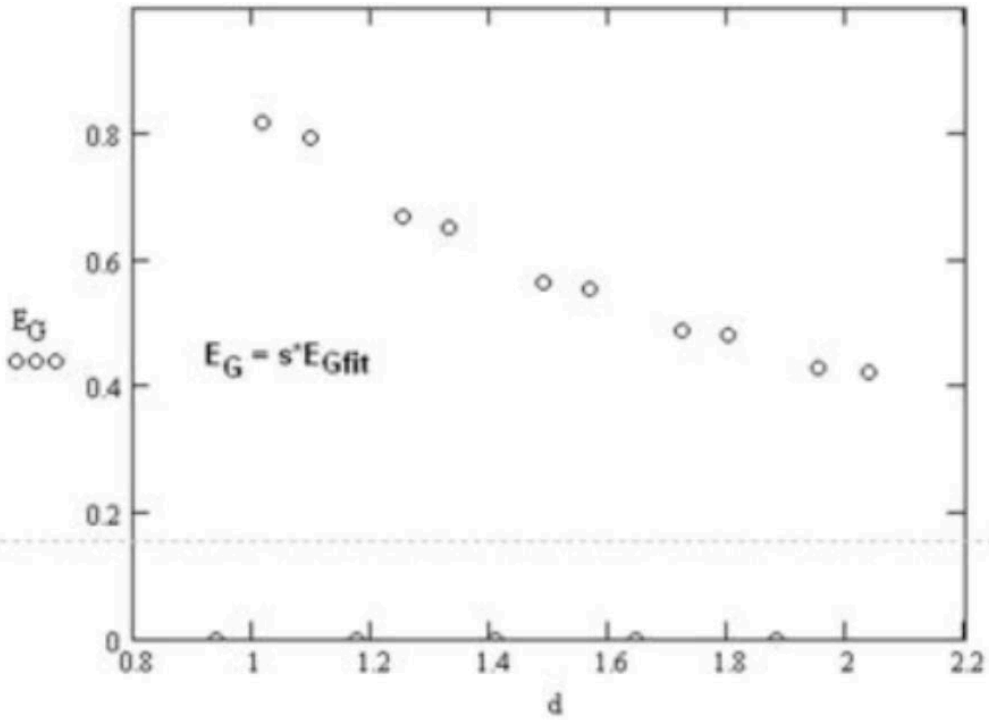
4b) Bandgap Versus Diameter: Plot



4d) Bandgap Versus Diameter: Fit







4d) Bandgap Versus Diameter: Fit

Constant resulting from n = 19: E_0 = .838eVnm