THEORITICAL STUDY OF THE STRUCTURAL, ELECTRONIC, ELECTRICAL & MECHANICAL PROPERTIES OF CARBON NANO RIBBON AND CARBON NANOTUBES

Engineer Reem Ghassan Shadeed

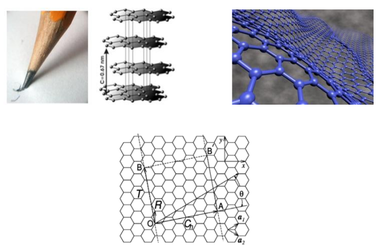
Jordan University : Master Thesis In Electrical Engineering Department

National Electric Power Company (NEPCO) : Head of Overhead Transmission Line Design Section

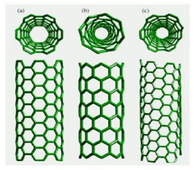
Abstract & Objectives

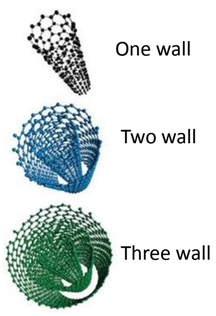
The purpose of this study is to investigate the unique physical properties and effects of changing the structur of

Carbon Nano Ribbon



Carbon Nanotubes CNT





PROPERTIES

Structural
Described using (n, m) Notation
ZigZag (n,0)
Armchair (n,n)
Chiral (m,n)

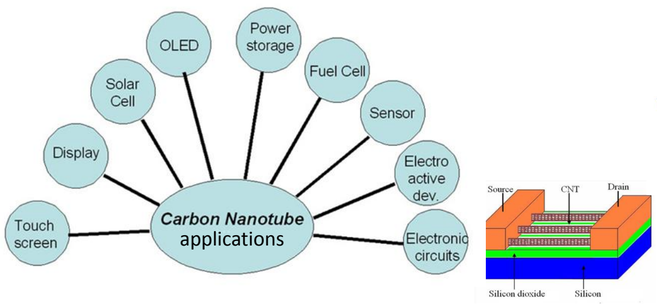
Electronic
P-CNTFET produces ~1500 A/m of the on-current per unit width which is **three times** the P-MOSFET produce at the same gate voltage

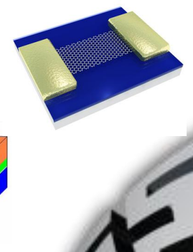
Electrical
Have the unique ability to be :
- insulators.
- Semiconductors.
- Conductors with conductivity up to 1000 times that of copper

Mechanical
Bent repeatedly up to 90^0

Density = 1/6 of steel density

Strength = 5 times steel strength



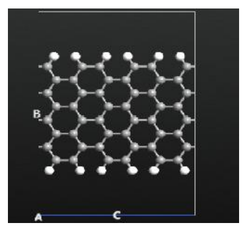


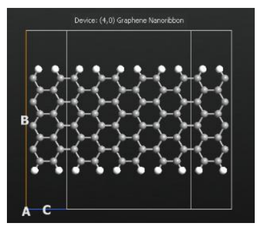
Future vision

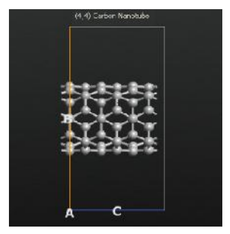
Nanotubes excellent strength to weight ratio creates the potential to build an elevator to space.

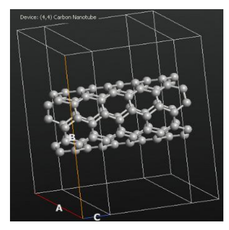
Materials & Methods

1) Build the Carbon Nanoribbon and the Carbon Nanotube



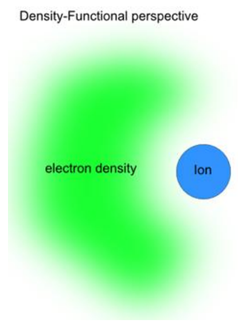






2) Edit the specification of the lattice parameter, coordinates of the elements, bulk configuration, operating temperature and all the required properties through the INPUT FDF file.

3) Relax the configuration using Density of Functional Theory (DFT) which is an approach to find a solution to the fundamental equation that describe the quantum behavior of atoms and also the molecules.



Done by siesta **Program**

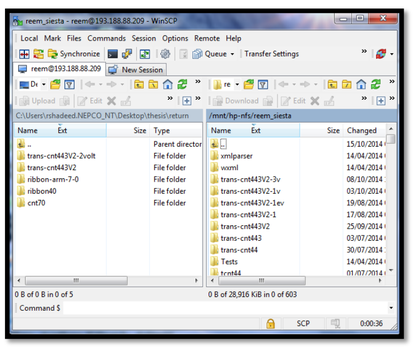
4) Analyze the Results from the output files.

Calculation Methods

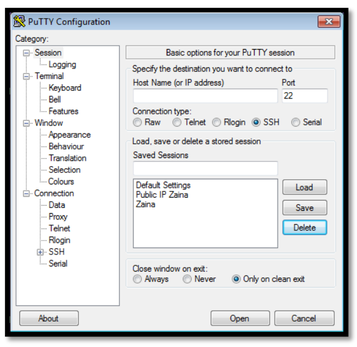
I am so proud to be one the First Users on Zaina Cluster

The Technical Team of **IMAN1** downloaded SIESTA , TRANSIESTA and TBTRANS program on **Zaina** Cluster to perform efficient electronic structure calculations and ab-initio molecular dynamics simulations of molecules and solids. They also downloaded the following programs on my personal computer to access the cluster remotely:

WinSCP to transfer and copy the needed files from my computer to **IMAN1** and vise versa



Putty (Secure SSH Client) to access the cluster securely and remotely from any location, control the input files, and run the simulations



For SCF (Self Consistent Field) number of iterations = 100 ~ 500

For number of iterations in relaxation (DM.NumGCsteps) = 100 ~ 500

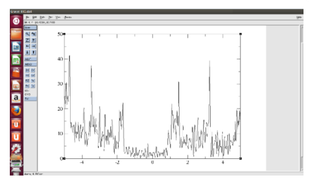
It takes **only four hours** for one hundred iterations on (4,4) CNT to relax on **IMAN1**, where it takes around **three thousand hours = 125 days** for the same amount of iterations on my personal computer

IMAN1

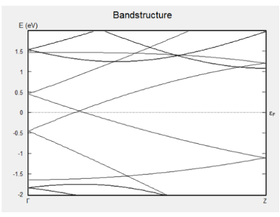
Without IMAN1 Supercomputer, this research cannot be completed

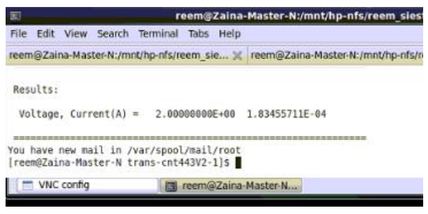
Results and Conclusion

Calculated and drew the **Density of State DOS** which describes the number of states per interval of energy at each energy level that are available to be occupied by electrons.

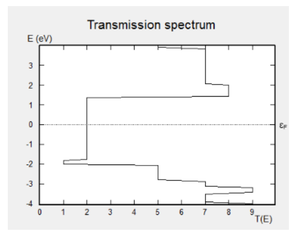


Calculated and drew the **Electronic Band Structure** which explain many physical properties of solids and describes those ranges of energy that an electron within the solid may have (called *energy bands*) and ranges of energy that it may not have (*Band Gap*)

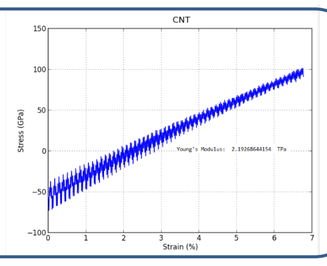




Drew the **Transmission Spectrum** which will be used to calculate the Electronic current density



Calculated the **Young Modulus of Elasticity** which describes the strength of mechanical properties of the materials and drew the Stress – Strain curve



All of these results are complied with the International results mentioned in the published papers