STRAIN INDUCED BAND GAPS IN GRAPHENE NANO RIBBONS

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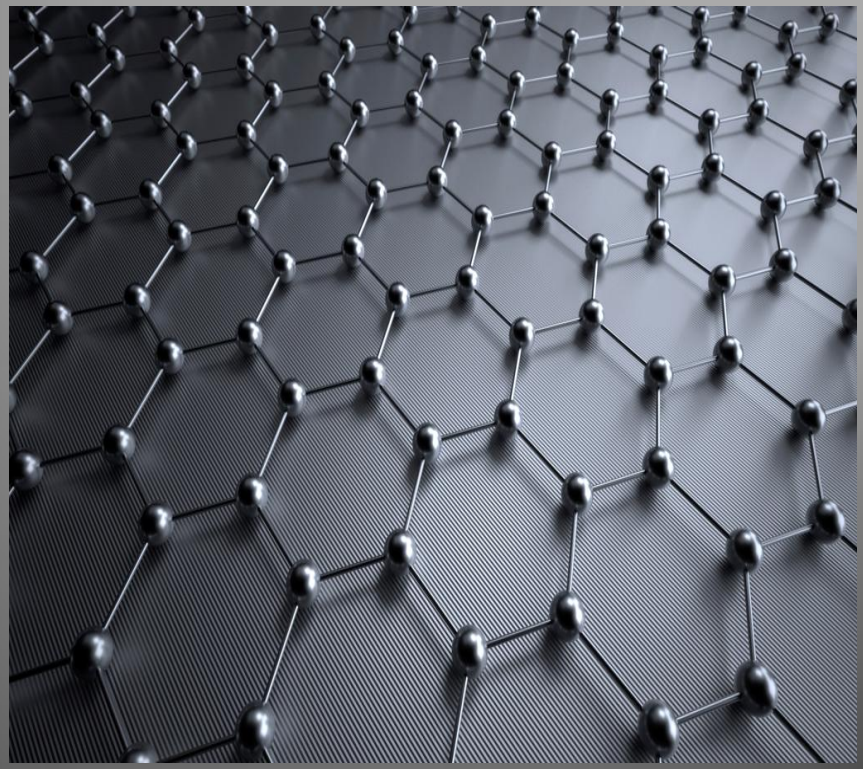
WHAT IS GRAPHENE?

- An allotrope of carbon
- Arranged in perfectly hexagonal lattice.
- Just one atom thick
- A 2-dimensional material.



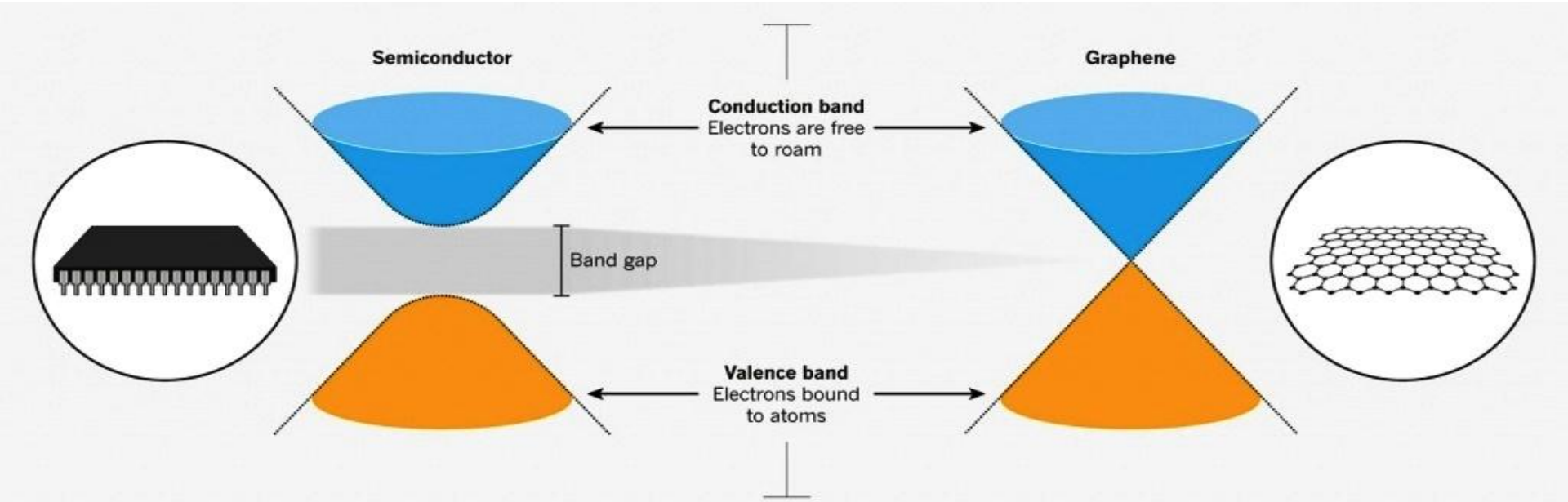
Remarkable properties…..

- Thinnest, lightest as well as strongest material known
- Conducts electricity better than almost any other material
- Extremely flexible
- Transmits almost 97.7 % of light
- The energy–momentum dispersion is linear in graphene leads to very high electron mobility
- Can be used in numerous applications as in automobile field, satellite navigation, medical field etc

Biggest Disadvantage:

Zero band gap:

- The conduction band touches the valence band at the Fermi level
- Therefore no threshold energy is required to move electrons from the conduction band to valence band.



- Due to zero band gap, there is no stoppage of electrons inside Graphene at applied gate voltage, which limits its application in the field of electronics.
- If we could open and tune the band gap, then graphene can be used as a semiconductor with great efficiency.

  Graphene Nano Ribbons (GNRs)….
- GNRs are 1-D graphene nanostructures with extremely thin width.
- Due to confinement of charge carriers, a band gap can be opened in Graphene Nano Ribbons.
- Two kinds of GNRs:

  a) ZIGZAG GNRs (ZGNRs)

  b) ARMCHAIR GNRs (AGNRs)

- **Aim of this project:**

  i) To tune band gap in ZGNRs with permissible strain

  ii) To observe corresponding change in its electronic properties

Tools

- We use DFT (Density Functional Theory) with VASP for theoretical band structure calculation.
- DFT deals with ground state energy as a functions of density of electrons.

Density Functional Theory

- To obtain approximate solution of many body Schrodinger equation
- Electronic ground state structure in terms of electronic density distribution

$$H\,\psi(x_1, x_2, \dots, x_N, R_1, R_2, \dots, R_M) = E\,\psi(x_1, x_2, \dots, x_N, R_1, R_2, \dots, R_M)$$

$$H = -\frac{1}{2m_e}\sum_i \nabla_i^2 - \frac{1}{2m_n}\sum_j \nabla_j^2 + \frac{1}{2}\sum_{\substack{i,k \\ i\neq k}} \frac{e^2}{r_i - r_k} + \frac{1}{2}\sum_{\substack{j,l \\ j\neq l}} \frac{Z_j Z_l e^2}{r_j - r_l} - \sum_{i,k} \frac{Z_i e^2}{r_i - r_k}$$

$$H = T_e + T_n + V_{ee} + V_{nn} + V_{en}$$

- Born-Oppenheimer approximation:

$$T_n = 0; V_{nn} = constant \Rightarrow$$

$$H = T_e + V_{ee} + V_{en}$$

- Kinetic energy can be approximated as a function of density such that

$$E(n, r) = F(n) + \int V_{ext}(r) n(r) dr + V_{ee}(r) + V_{en}(r)$$

- DFT uniquely determines the ground state energy by minimizing the energy and by playing with the density.

- **VASP** (***Vienna Ab Initio Simulation Package)***.
- **Input parameters**:

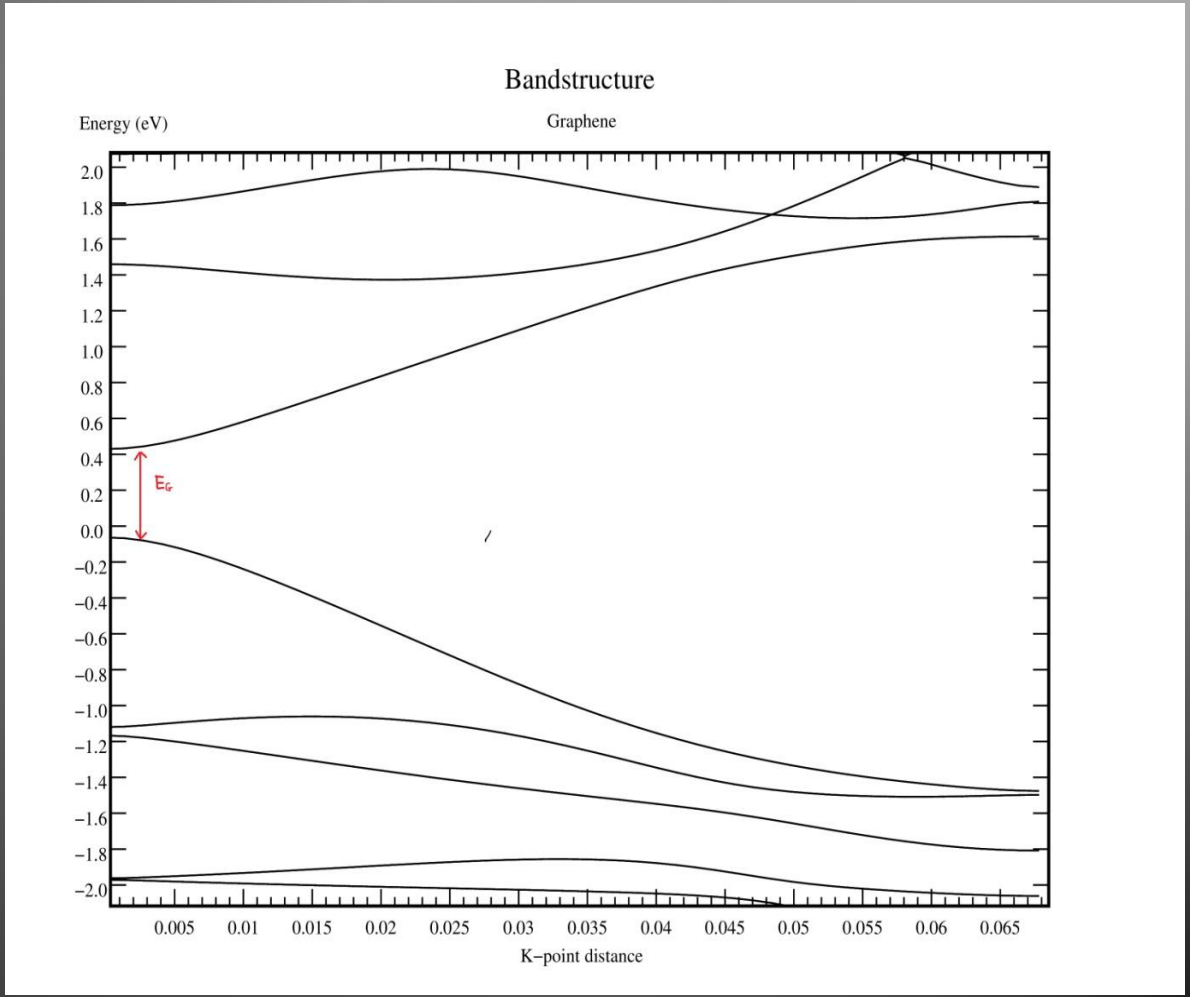
1. **INCAR**: central input file of VASP contains input parameters, which determines what to do and how to do.
2. **POSCAR**: it contains the positions of the ions;
3. **KPOINTS**: it contains K Points in k-points coordinates.
4. **POTCAR**: this file contains potentials and information about atoms, their masses, valence electrons.

- **Calculations**……

1. **Relaxation**: an optimization step, to relax the structure.
2. **Self consistent calculation**: this step provides the charge density and the free energy of the system.
3. **Non self consistent calculation**: using the charge density provided by second step, this step calculates the band structure.

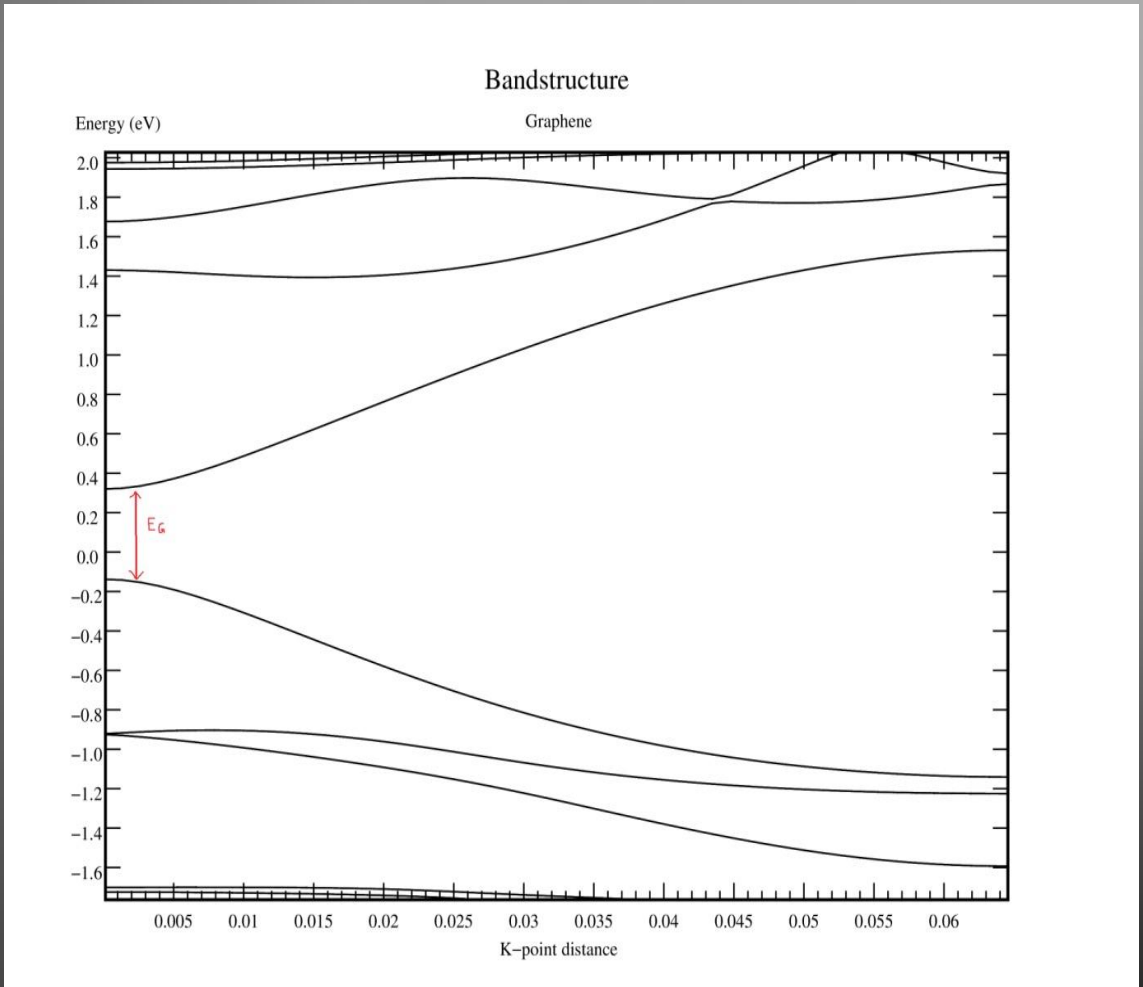
OBSERVATIONS:

- 3-ZGNRs
- 0% strain (original state):
- band gap between lowermost valance band and uppermost conduction band near the Fermi level is present (semi conducting)



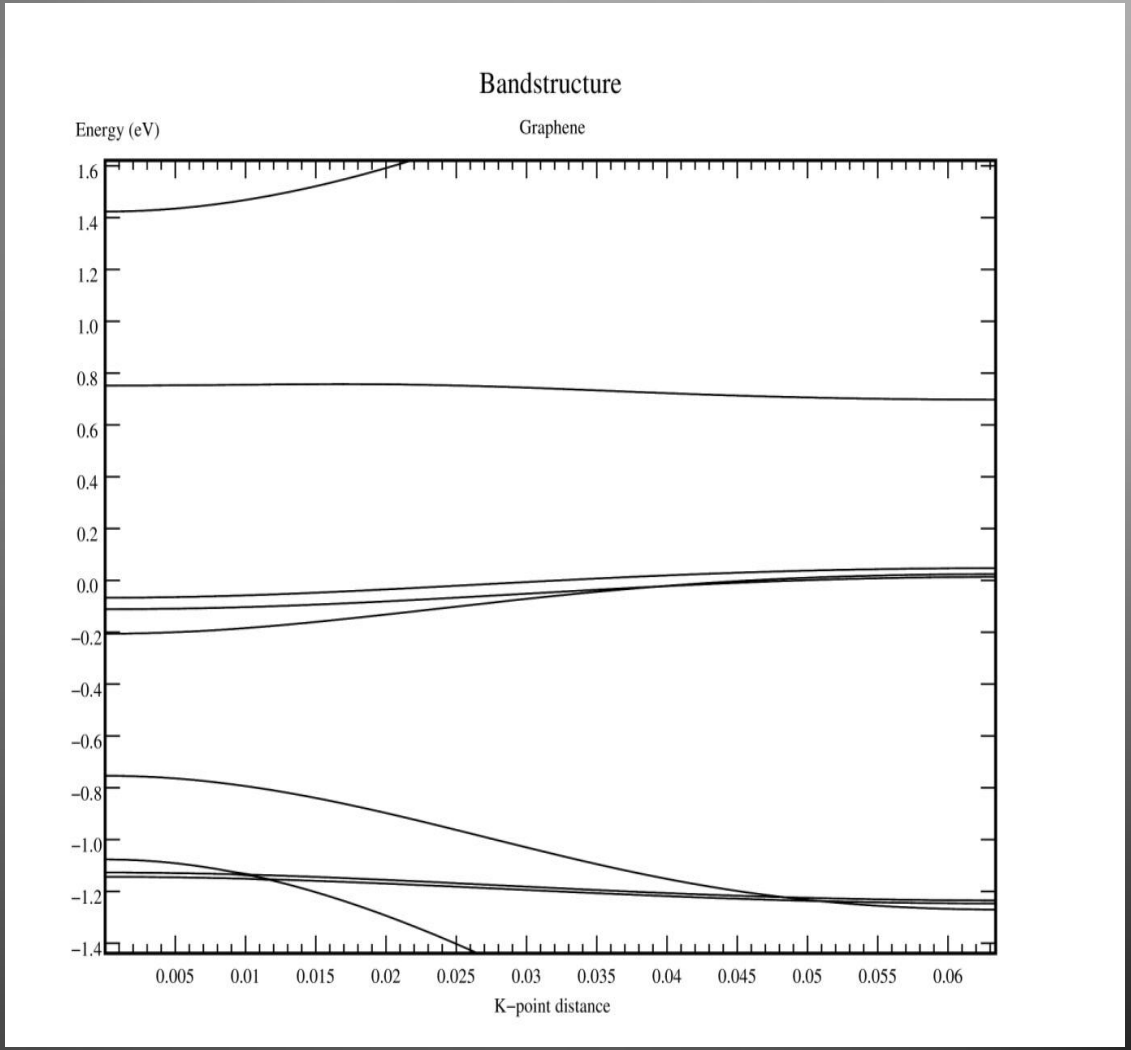
OBSERVATIONS:

- 3-ZGNRs at 5% strain:
- Still a band gap is present at the Fermi level, possesses semi conducting nature



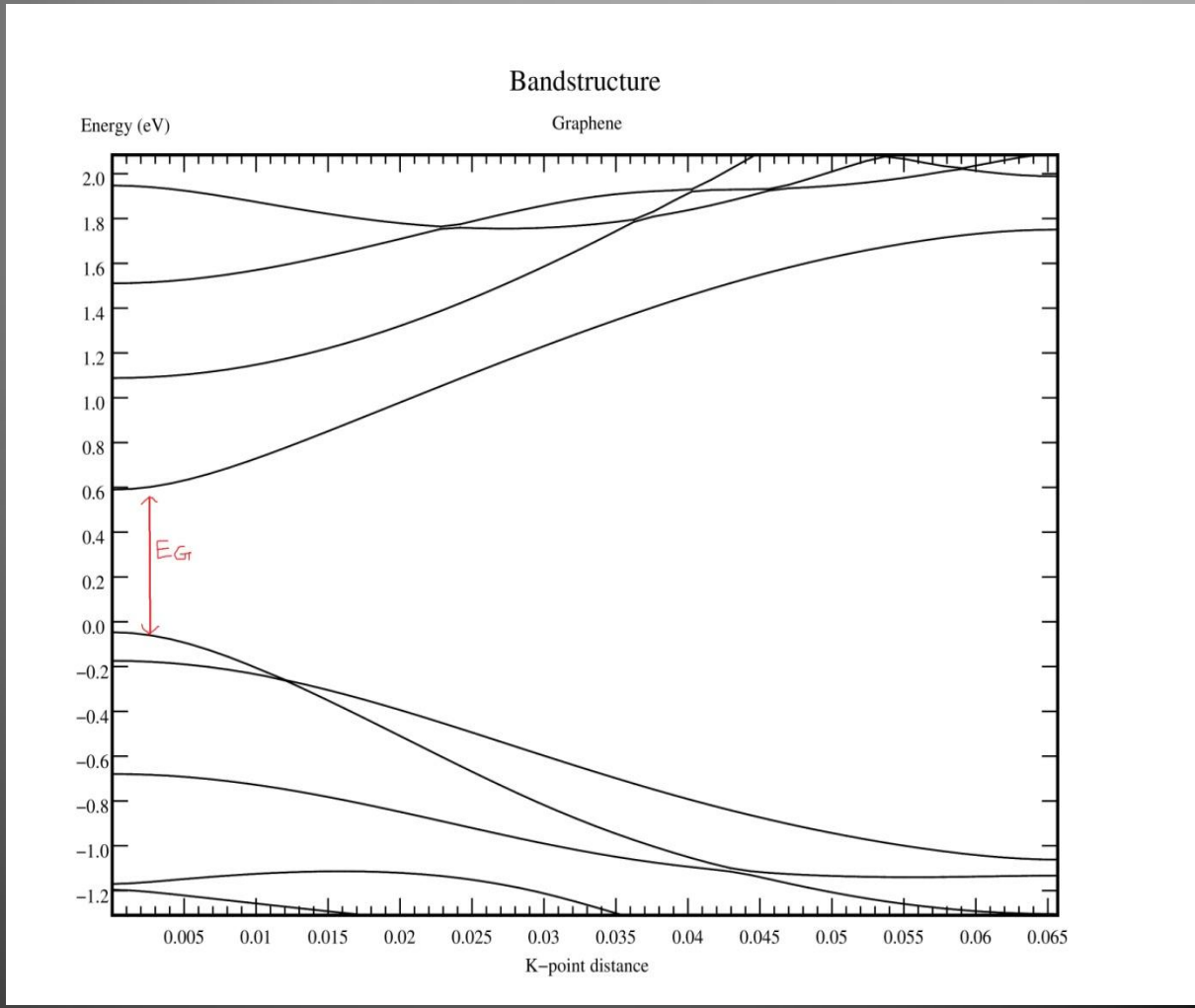
OBSERVATIONS:

- 3-ZGNRs at 6% strain and beyond:
- At Fermi level the lowermost conduction band and uppermost valance band overlap. This shows the metallicity of GNRs.



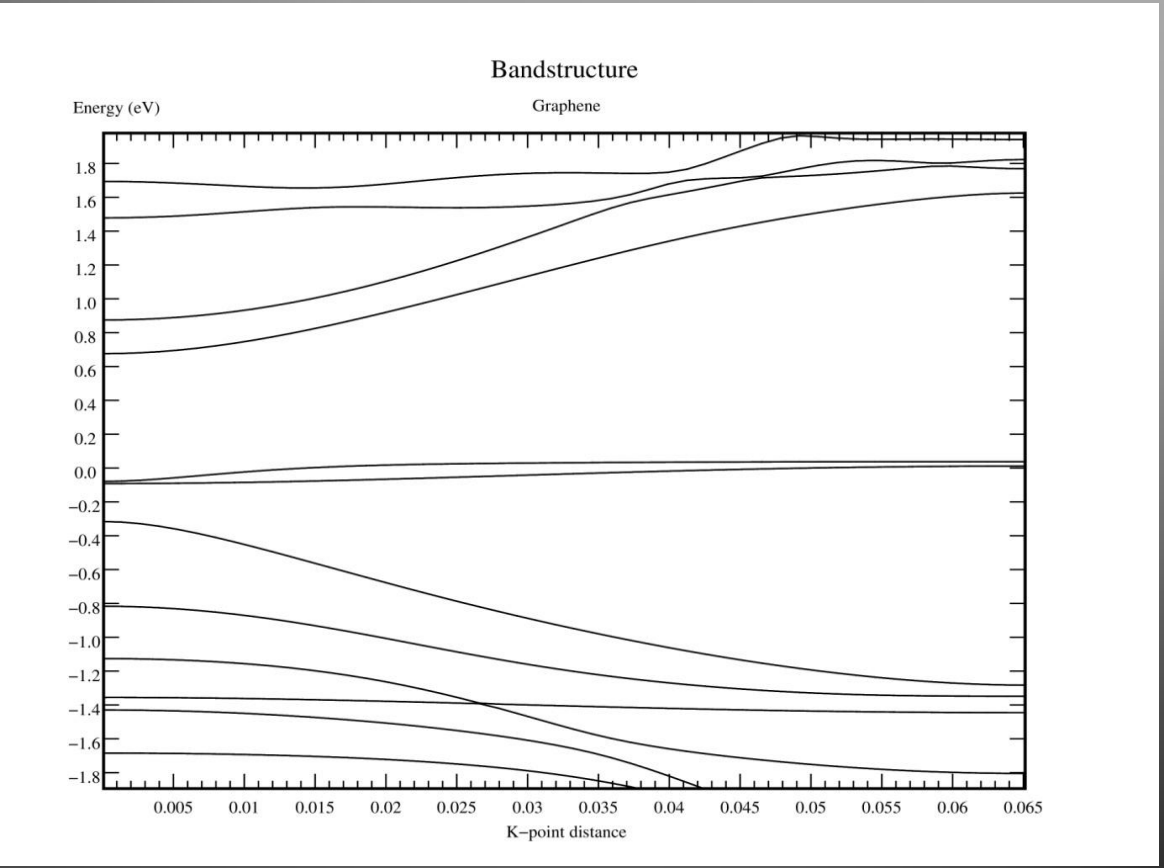
OBSERVATIONS:

- 6-ZGNRs at 3% strain:
- A band gap is present at the Fermi level, possesses semi conducting nature.



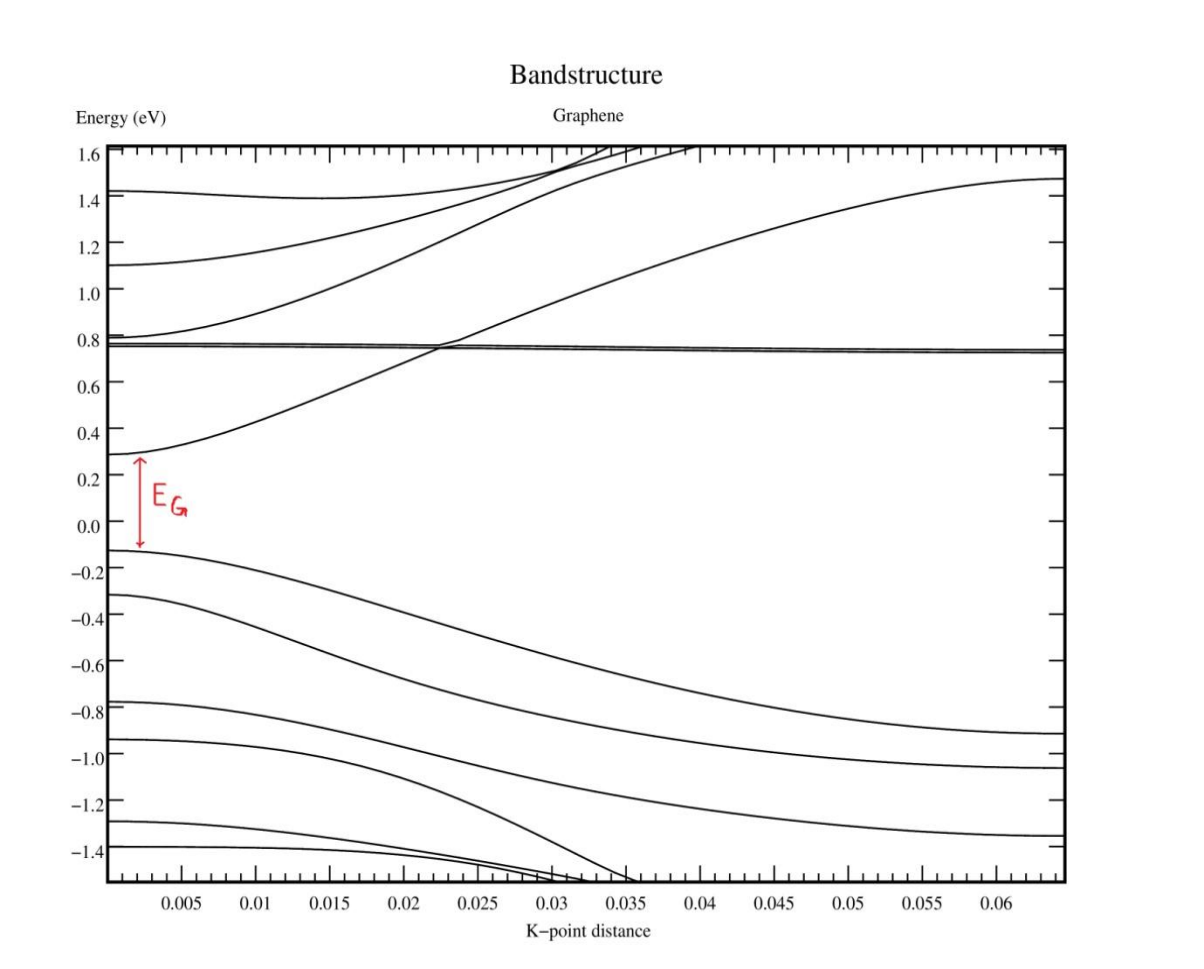
OBSERVATIONS:

- 6-ZGNRs at 4% strain and beyond:
- At Fermi level the lowermost conduction band and uppermost valance band overlap, metallic characters.



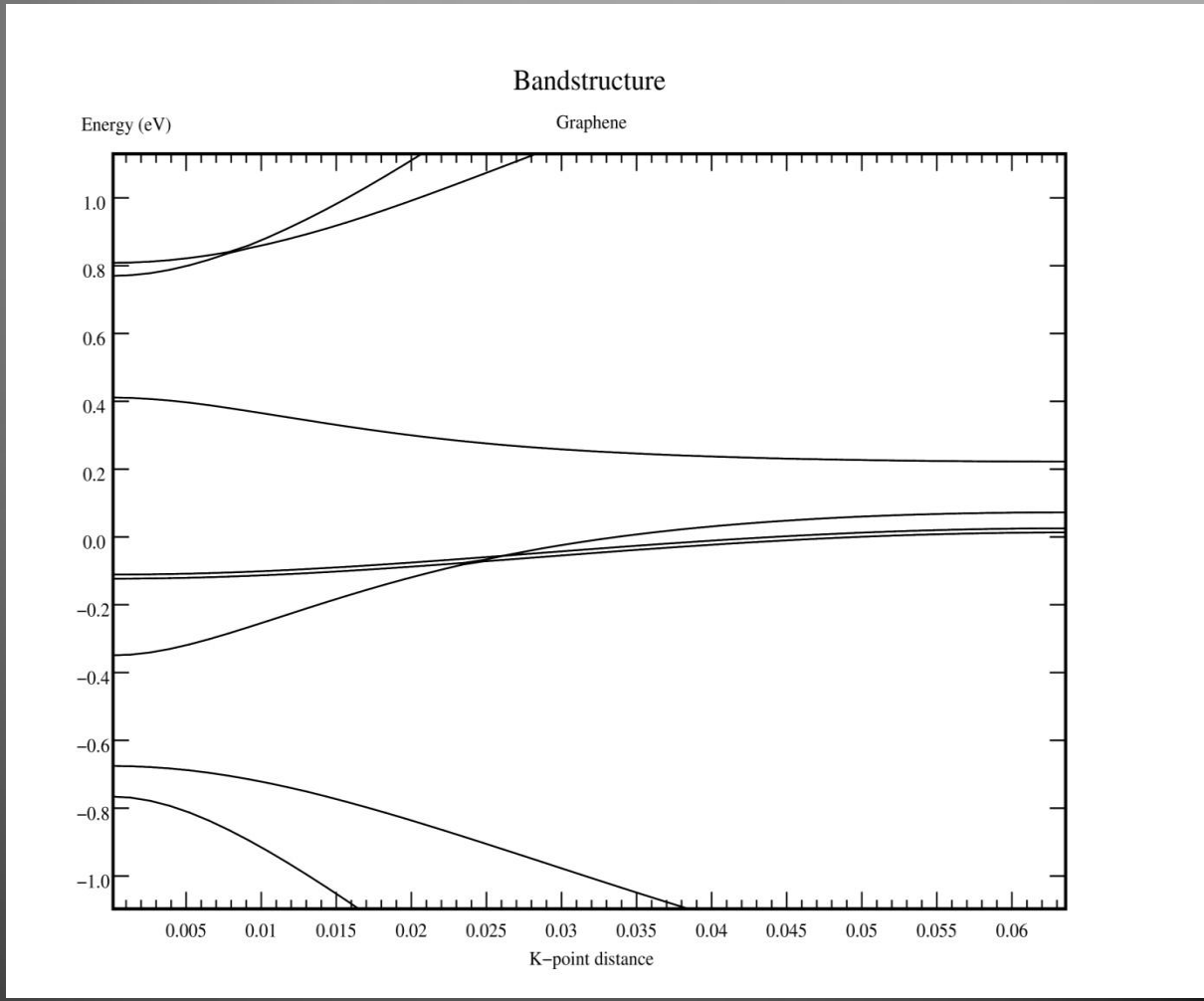
OBSERVATIONS:

- 8-ZGNRs at 5% strain :
- A band gap is present at the Fermi level, showing semiconducting nature.



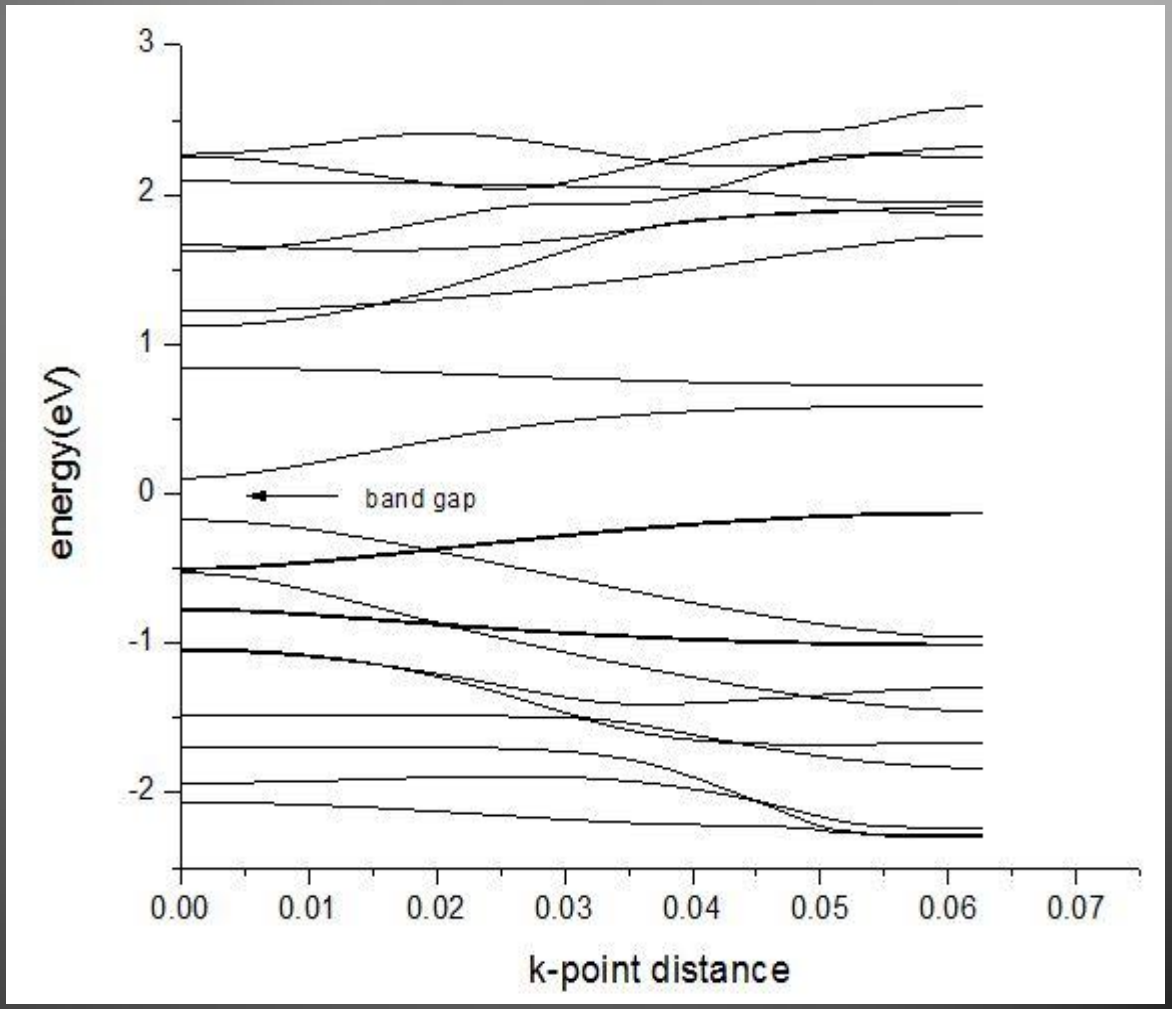
OBSERVATIONS:

- 8-ZGNRs at 6% strain:
- At Fermi level the lowermost conduction band and uppermost valance band overlap, metallic character.

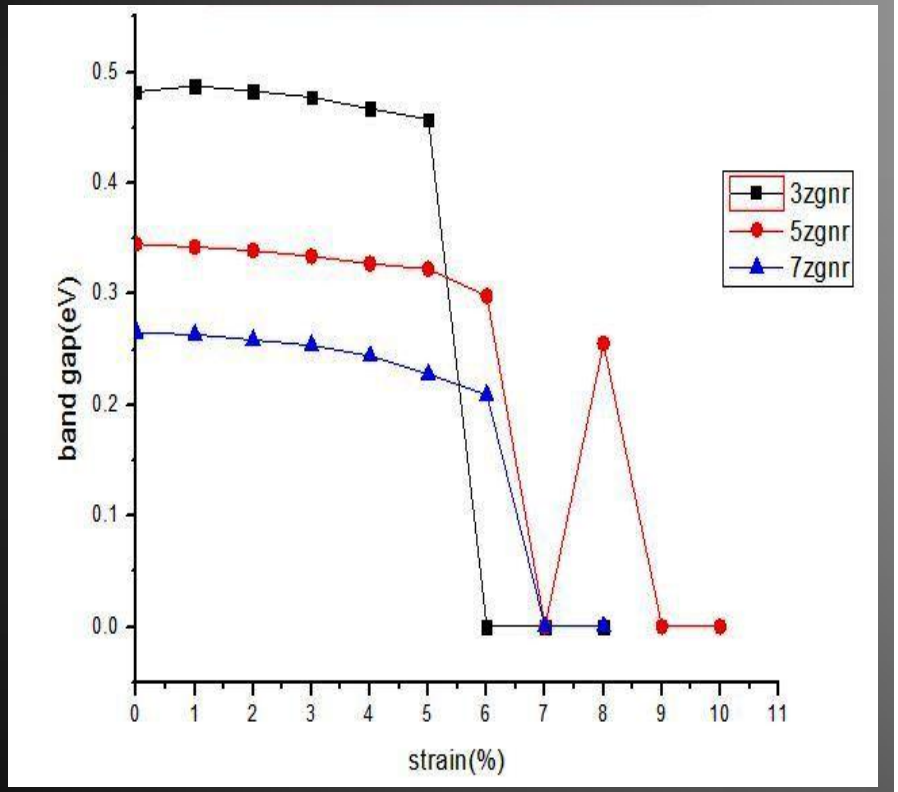


OBSERVATIONS:

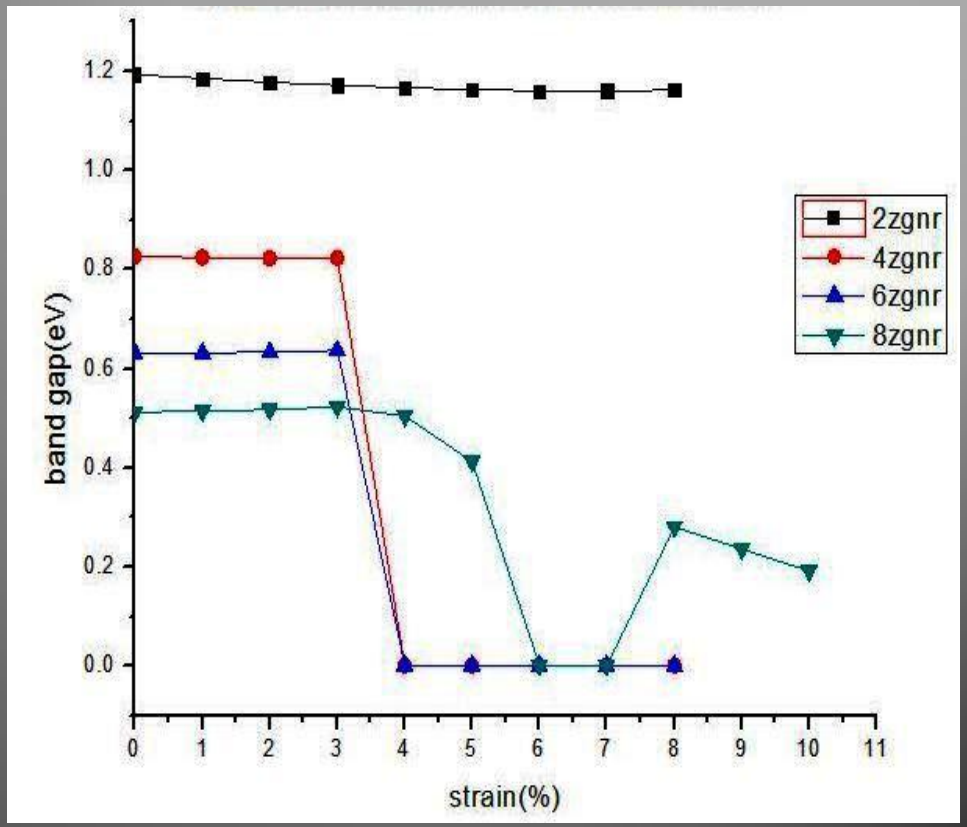
- 8-ZGNRs at 8% strain:
- There is again a band gap present at the Fermi level. It tells that the character has again shifted to semiconducting nature.



Band gap magnitude:



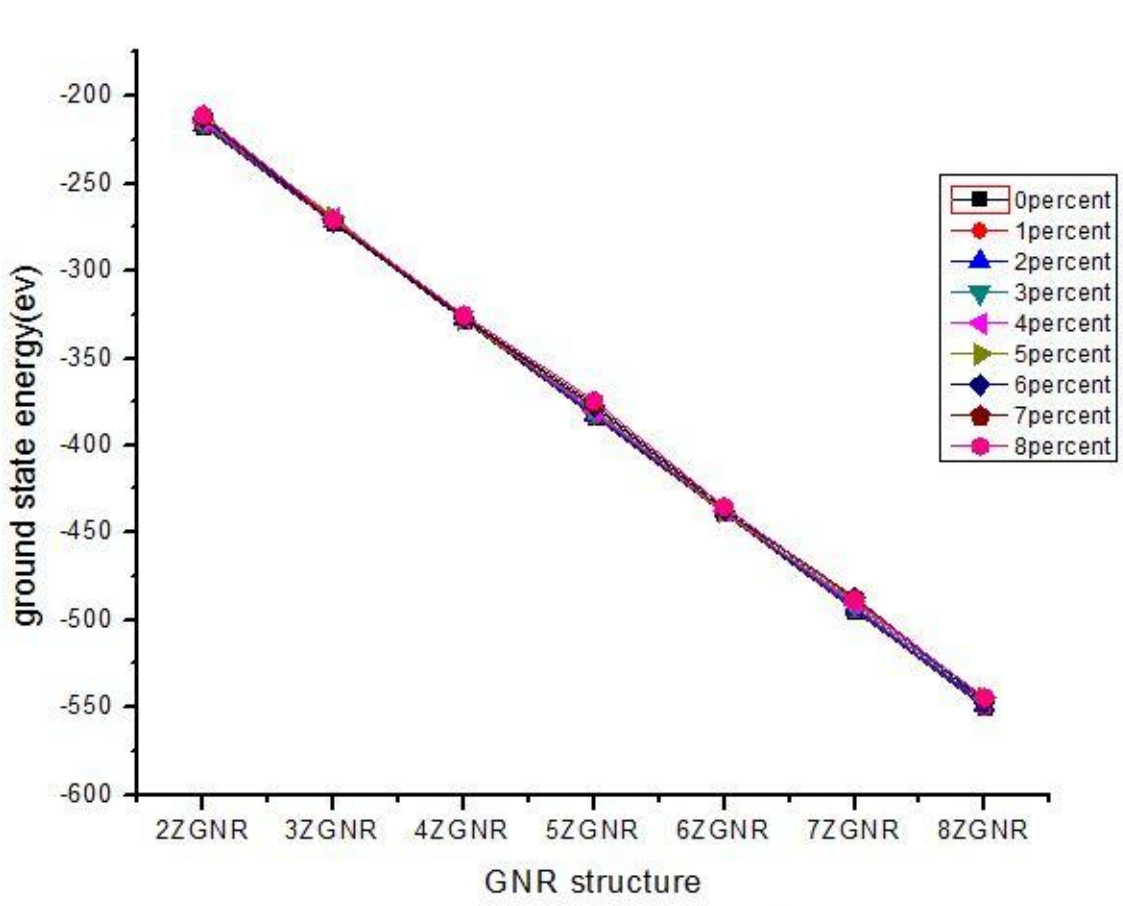
Odd-ZGNRs



Even-ZGNRs

Ground state energy for ZGNRs under strain

- The relationship is linear between all these 7 ZGNRs.
- For a particular ZGNR, the ground state energy remains almost constant under all different strains applied.



ground state energy for GNR files for different strain

TABLE I : *Band gaps created by the strain in the GNRs (eV)* :

Strain GNRs	0%	1%	2%	3%	4%	5%	6%	7%	8%
2-ZGNR	1.1938	1.1863	1.1785	1.1723	1.1671	1.1635	1.161	1.1613	1.31621
3-ZGNR	0.4826	0.4877	0.483	0.4777	0.4671	0.4575	0	0	0
4-ZGNR	0.8262	0.8238	0.8224	0.8233	0	0	0	0	0
5-ZGNR	0.3451	0.3423	0.3391	0.334	0.3274	0.3224	0.2983	0	0.2552
6-ZGNR	0.6311	0.6311	0.6314	0.6333	0.6364	0	0	0	0
7-ZGNR	0.2651	0.2636	0.2586	0.2536	0.2536	0.2277	0.2089	0	0
8-ZGNR	0.5124	0.5141	0.5171	0.523	0.523	0.4127	0	0	0.2804

CONCLUSIONS:

- Electronic properties of graphene nano ribbons can be controlled by inducing strain on the GNRs.
- Metallic and semiconducting behaviour of GNRs can be altered by inducing strain.
- Controlling of band gaps in GNRs can be very useful for the semiconductor industry.

THANK YOU !!