Energy Band-Gap Engineering of Graphene-Derived Nanostructures

Nick Woods

nw637@york.ac.uk

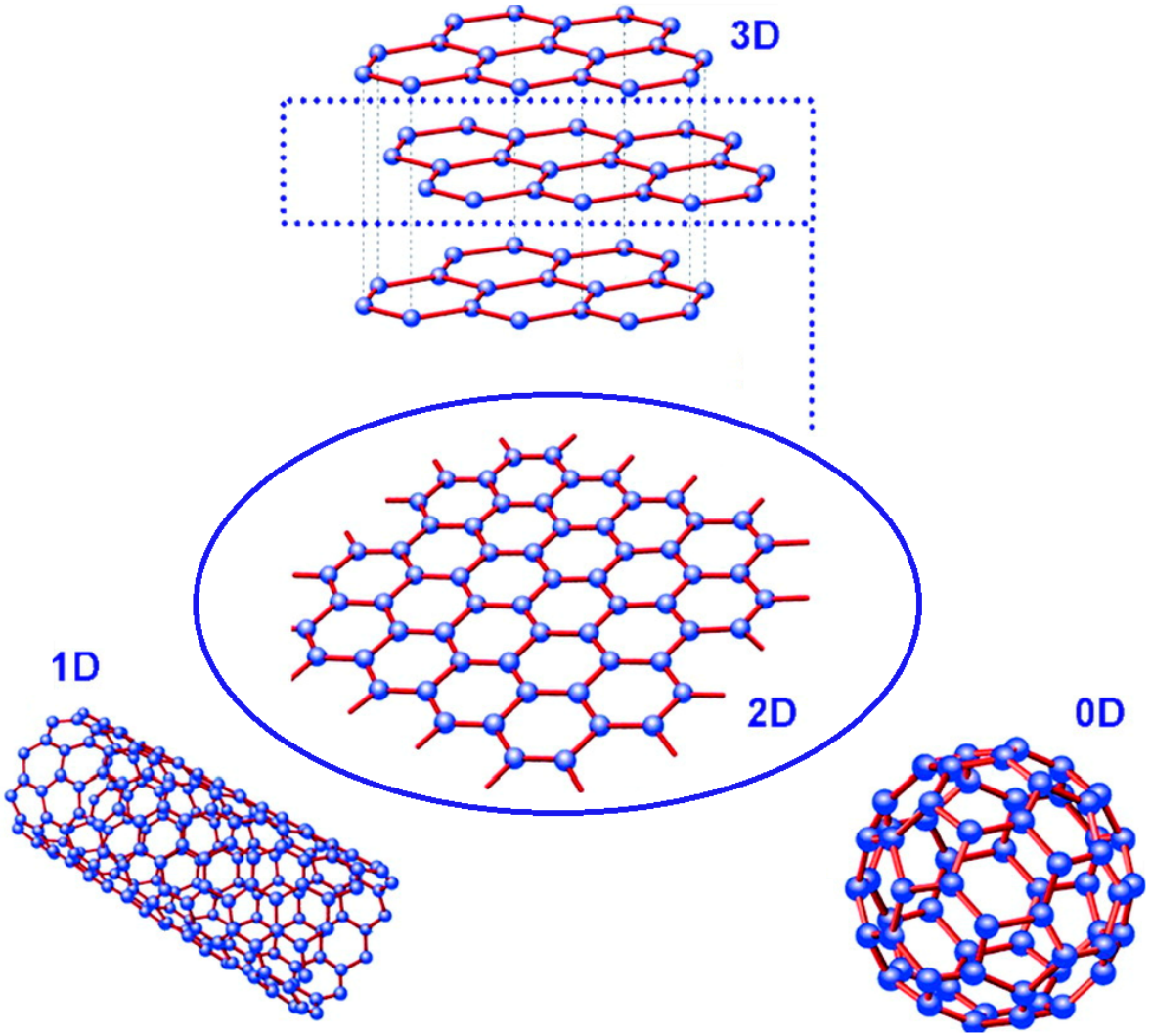
Supervisor: Dr. Yvette Hancock

June 3, 2015

Overview

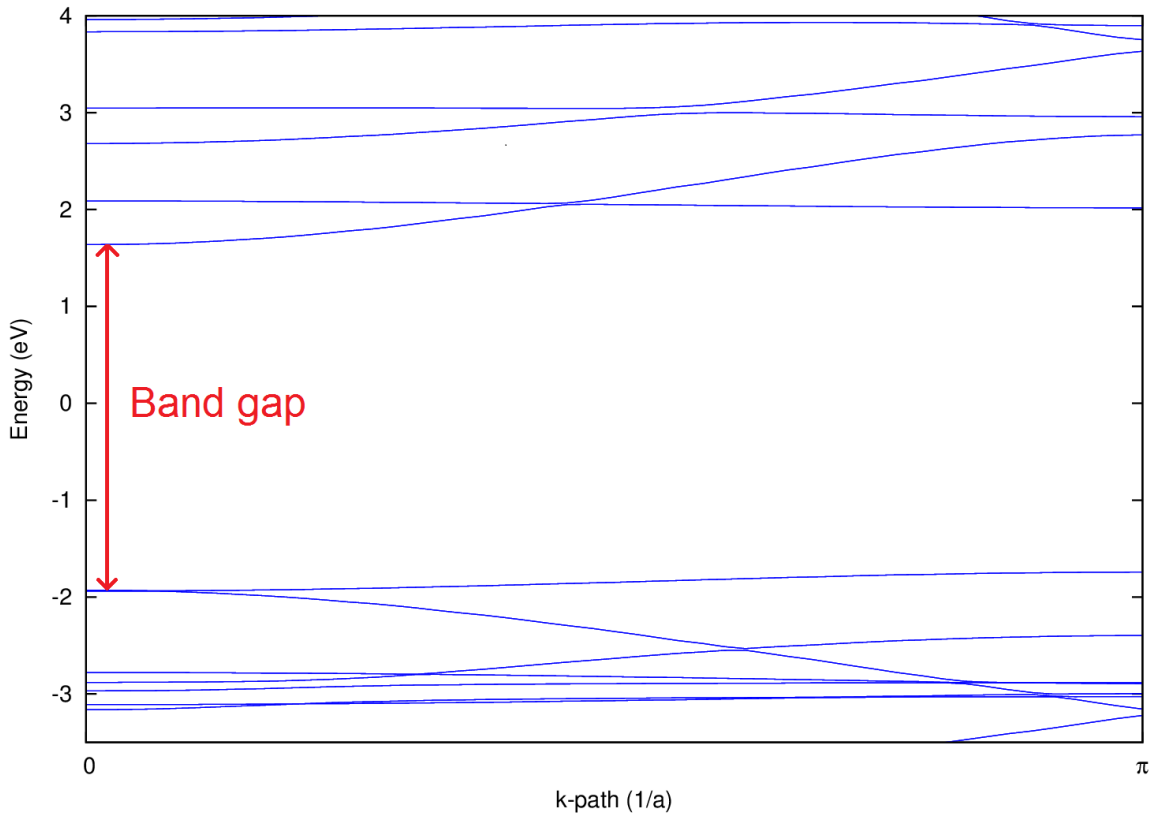
Introduction

- What is Graphene?



Research Question

- How can the band-gap of graphene be modified in a useful way?



Motivation

- Semiconductors play a huge role in the electronics industry (e.g. transistors).

Motivation

- Semiconductors play a huge role in the electronics industry (e.g. transistors).
- Computer processors can have in excess of one billion transistors.

Motivation

- Semiconductors play a huge role in the electronics industry (e.g. transistors).
- Computer processors can have in excess of one billion transistors.
- Why Graphene?

Theoretical Techniques

Density Functional Theory

Tight-Binding Model

Theoretical Techniques

Density Functional Theory

- *Ab initio* technique.

Tight-Binding Model

- A model (not a theory).

Theoretical Techniques

Density Functional Theory

- *Ab initio* technique.
- Long computation times.

Tight-Binding Model

- A model (not a theory).
- Short computation times.

Theoretical Techniques

Density Functional Theory

- *Ab initio* technique.
- Long computation times.

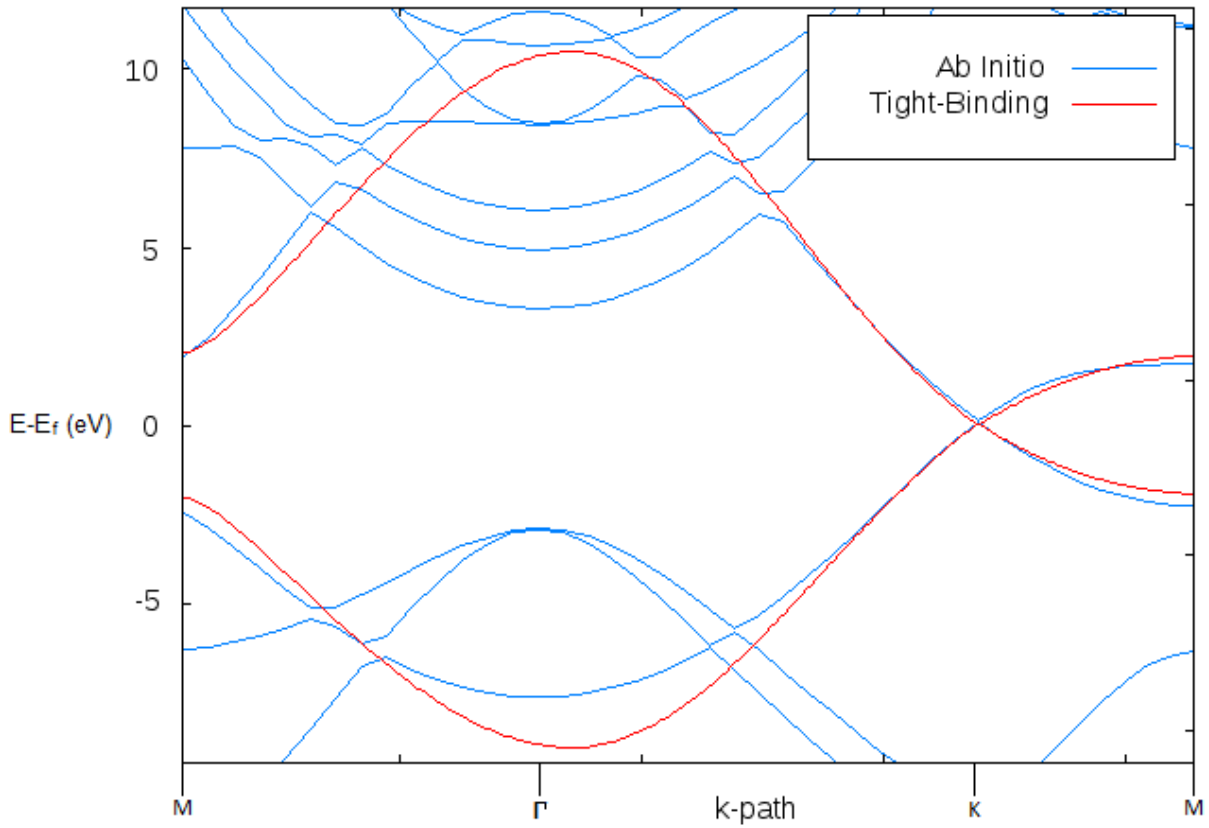
Tight-Binding Model

- A model (not a theory).
- Short computation times.

Strategy: Use density functional theory to parametrise the tight-binding model.

Bulk Graphene

- Bulk graphene has no band gap.

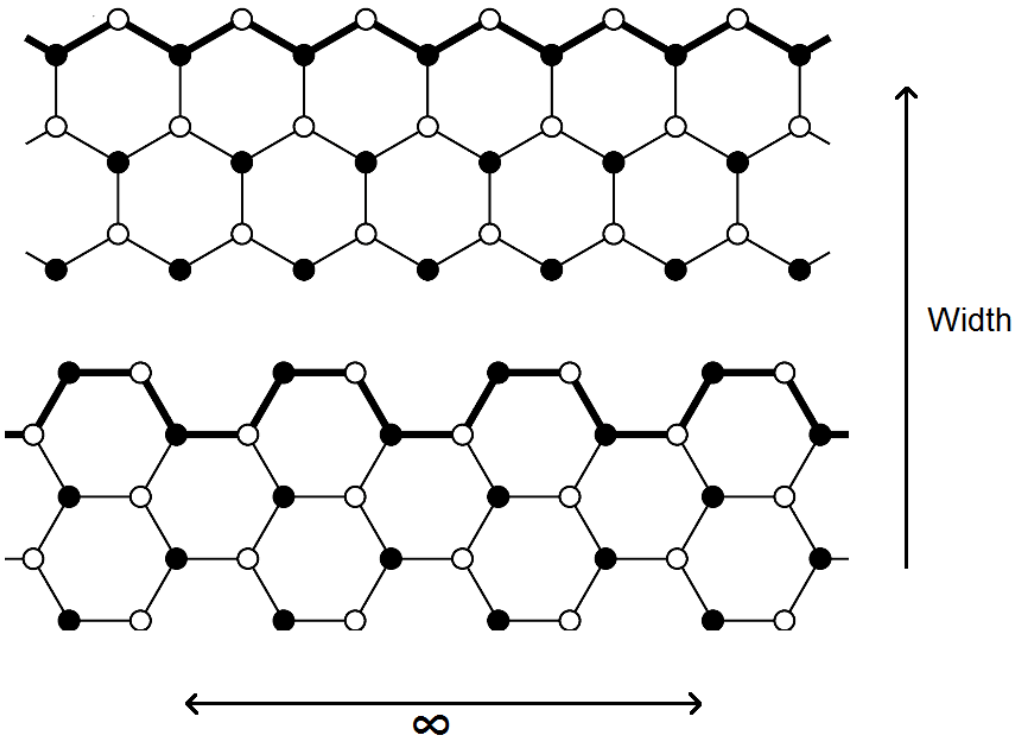


Techniques to Alter the Band-Gap

- Introduce strain.

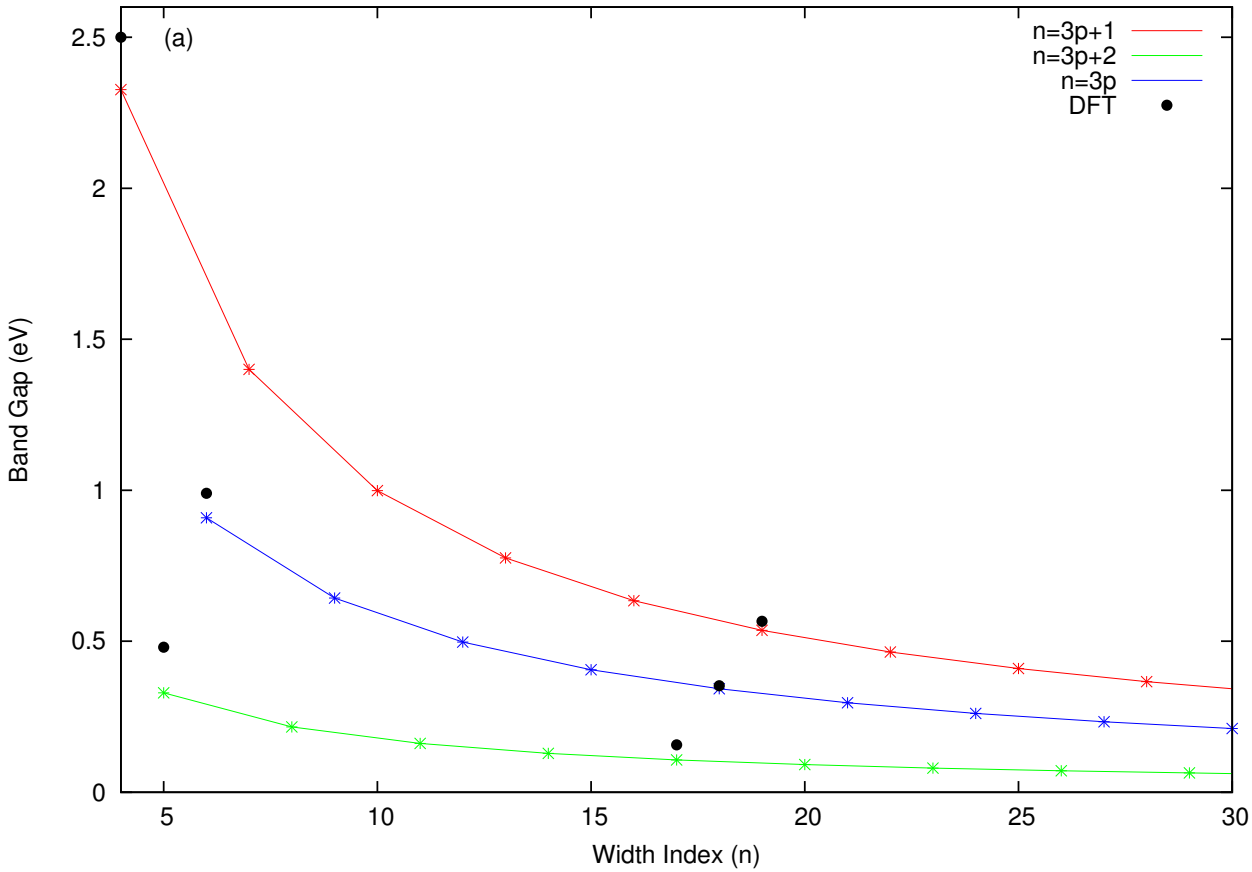
Techniques to Alter the Band-Gap

- Introduce strain.
- Pattern two-dimensional graphene sheets into quasi-one-dimensional graphene nanoribbons (GNRs).



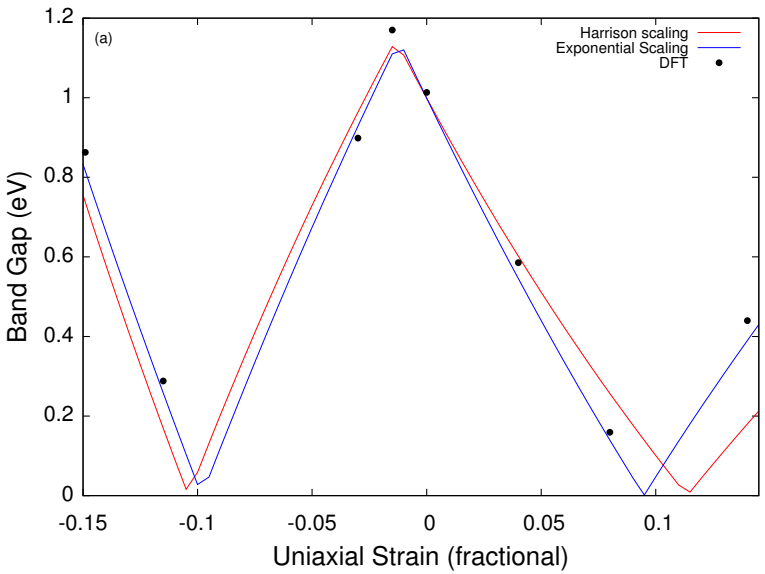
Graphene Nanoribbons

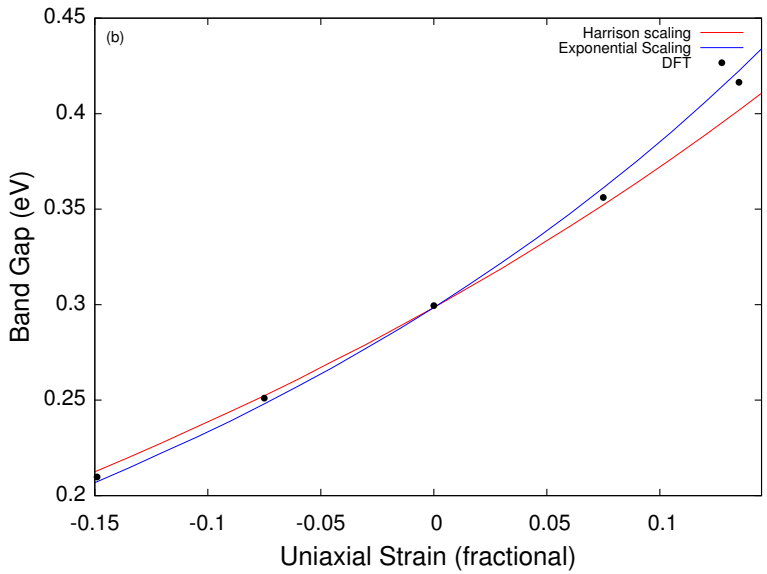
- Large range of band-gaps available to GNRs by increasing the width alone.



Strained GNRs

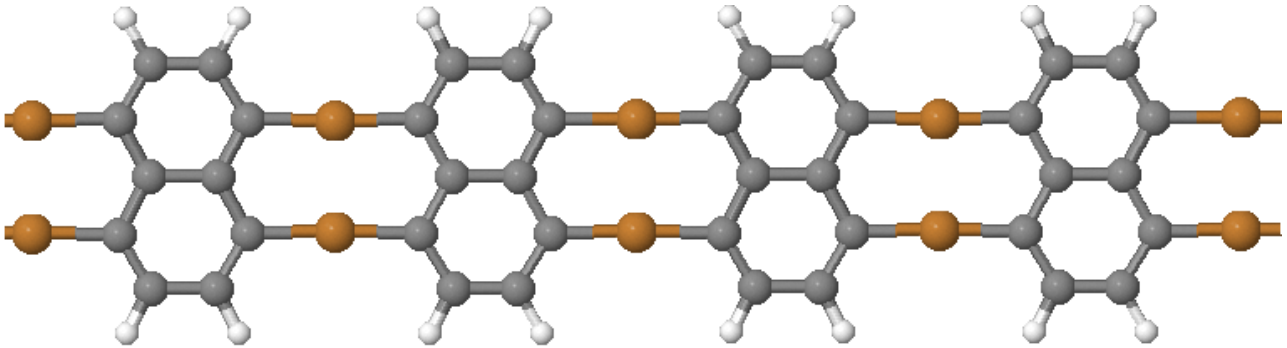
- Uniaxial strain is able to increase and decrease the band-gap in (a) armchair-edged graphene nanoribbons and (b) zigzag-edged graphene nanoribbons.





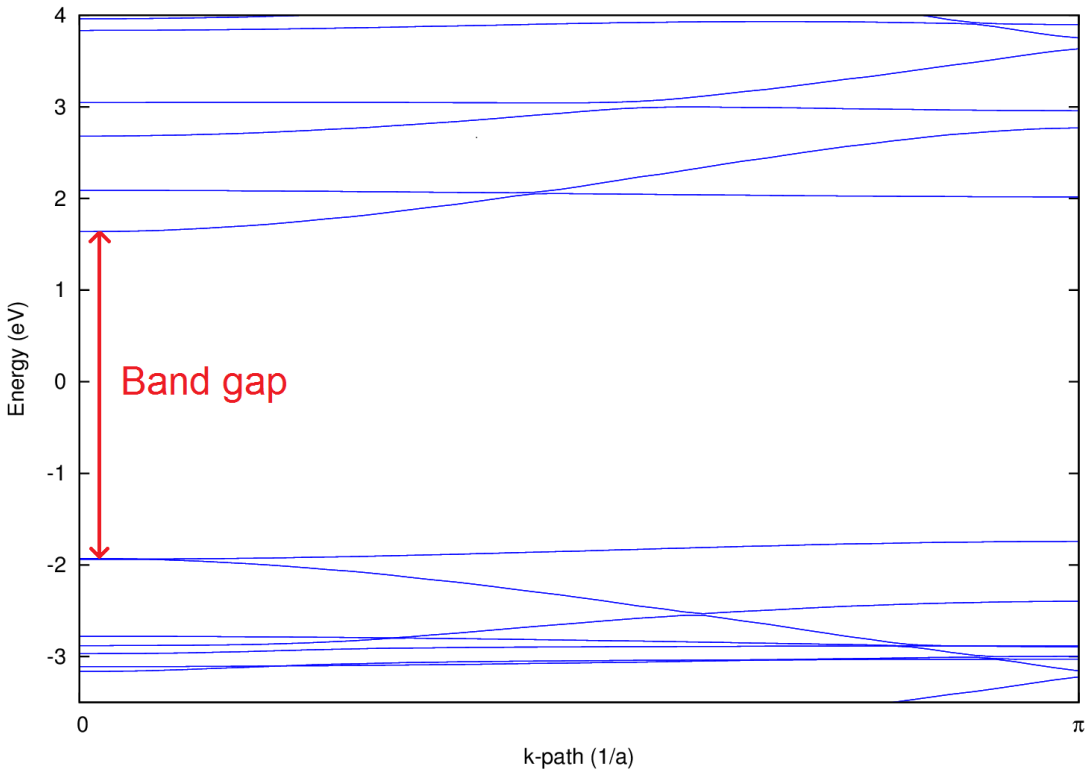
Foreign Species within GNRs

- Change the geometrical structure of GNRs by introducing periodic copper connections (orange).



Foreign Species within GNRs

- Only the smallest width copper-GNR is a semiconductor.



- The rest are metallic.

Conclusions

- Bulk graphene does not posses an inherent band gap - despite an applied uniaxial strain.

Conclusions

- Bulk graphene does not posses an inherent band gap - despite an applied uniaxial strain.
- Patterning graphene into quasi-one-dimensional GNRs allows for a large range of band-gaps to be realised.

Conclusions

- Bulk graphene does not posses an inherent band gap - despite an applied uniaxial strain.
- Patterning graphene into quasi-one-dimensional GNRs allows for a large range of band-gaps to be realised.
- Positions GNRs well for use in next-generation nanoelectronics.

Further Work

- Band-gaps are not the only feature of a successful semiconductor.
- What other properties do strained or doped GNRs posses?
  - Electron transport calculations.

The End

Questions?