Band-Gap Engineering of Graphene

Energy Band-Gap Engineering of Graphene-Derived Nanostructures

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Overview

Band-Gap Engineering of Graphene

Overview

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- 1 Introduction
 - What is graphene?
 - Research question and motivation.
- 2 Theory
- 3 Results
- 4 Conclusion

Introduction

Band-Gap Engineering of Graphene

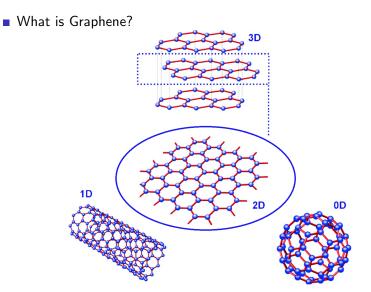
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Research Question

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Introduction

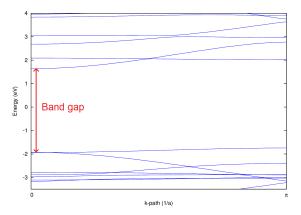
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How can the band-gap of graphene be modified in a useful way?



Motivation

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

Motivation

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

Computer processors can have in excess of one billion transistors.

Motivation

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

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Density Functional Theory

Tight-Binding Model

Density Functional Theory

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■ *Ab initio* technique.

Tight-Binding Model

A model (not a theory).

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Density Functional Theory

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Ab initio technique.

Long computation times.

Tight-Binding Model

A model (not a theory).

Short computation times.

Theory

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Density Functional Theory

- Ab initio technique.
- Long computation times.

Tight-Binding Model

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

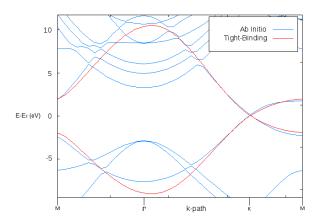
Strategy: Use density functional theory to parametrise the tight-binding model.

Bulk Graphene

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Theory

■ Bulk graphene has no band gap.



Techniques to Alter the Band-Gap

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Introduce strain.

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Techniques to Alter the Band-Gap

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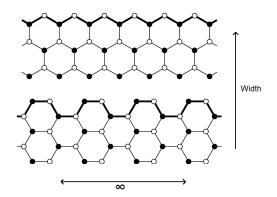
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- Introduce strain.
- Pattern two-dimensional graphene sheets into quasi-one-dimensional graphene nanoribbons (GNRs).



Graphene Nanoribbons

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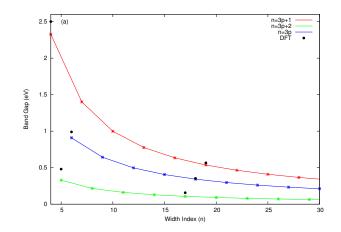
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■ Large range of band-gaps available to GNRs by increasing the width alone.



Strained GNRs

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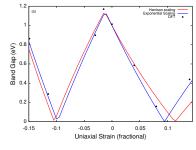
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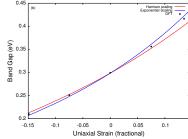
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 Uniaxial strain is able to increase and decrease the band-gap in (a) armchair-edged graphene nanoribbons and (b) zigzag-edged graphene nanoribbons.





Foreign Species within GNRs

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Results

■ Change the geometrical structure of GNRs by introducing

periodic copper connections (orange).



Foreign Species within GNRs

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Overview

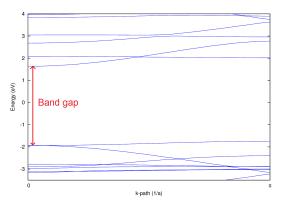
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• Only the smallest width copper-GNR is a semiconductor.



The rest are metallic.

Conclusions

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

Conclusions

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Conclusion

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

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- 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

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Conclusion

 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

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Questions?