In-silico design of an all-armchair graphene nanoribbon field effect transistor (GNRFET) sensor for the detection of starch

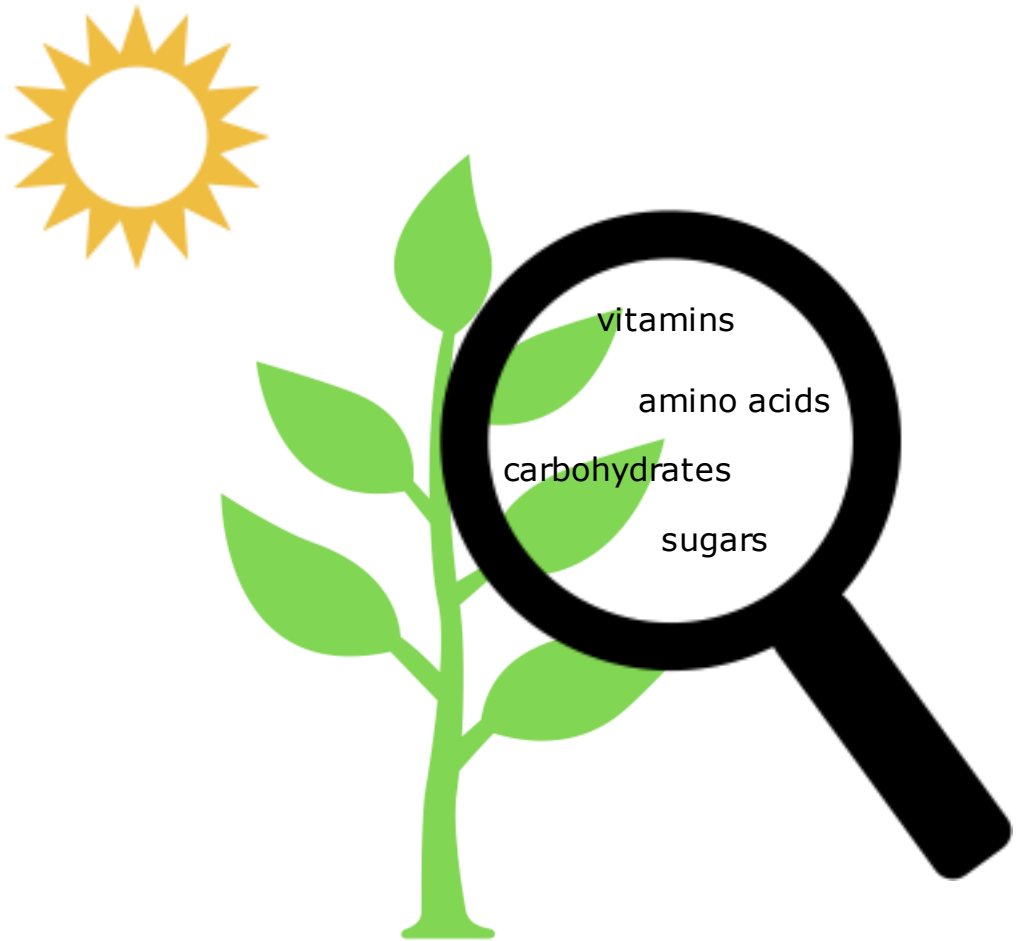
Isabella López-Cifuentes, Andrés Jaramillo-Botero, PhD.

ilopez11@javerianacali.edu.co ajaramil@javerianacali.edu.co

Outline

1. Motivation
2. Field effect transistors and graphene
3. Design process
   - Functionalization
   - Geometry and IV characteristics
4. Conclusions

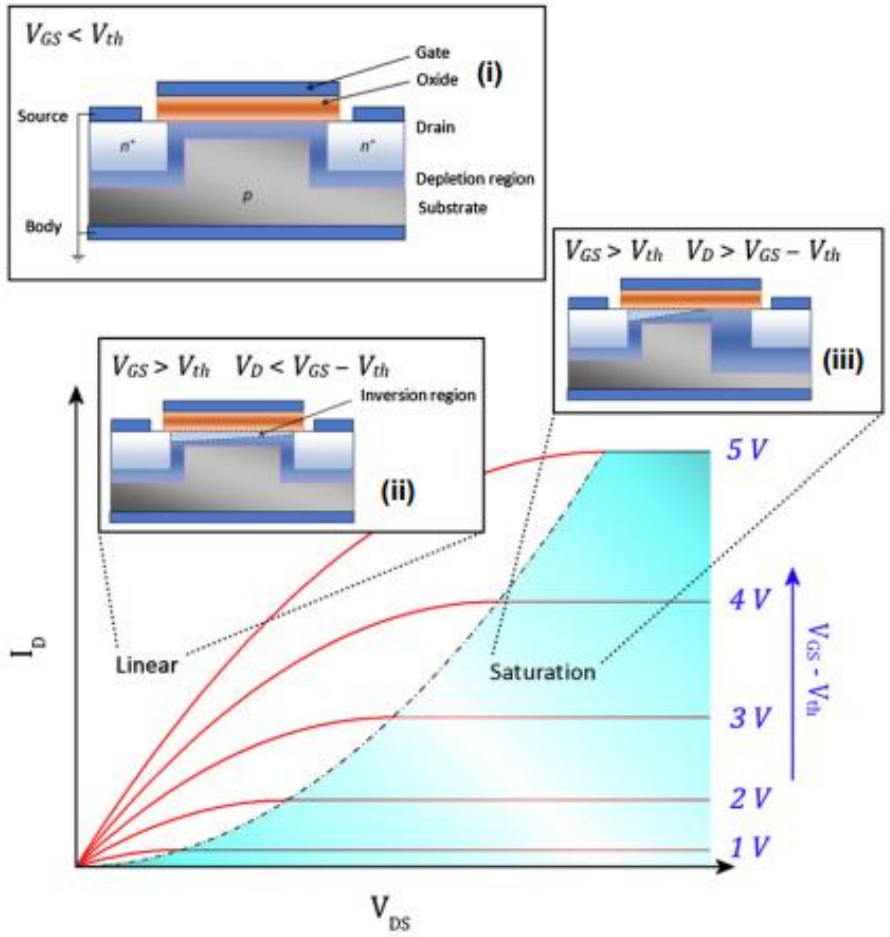
Motivation



Motivation

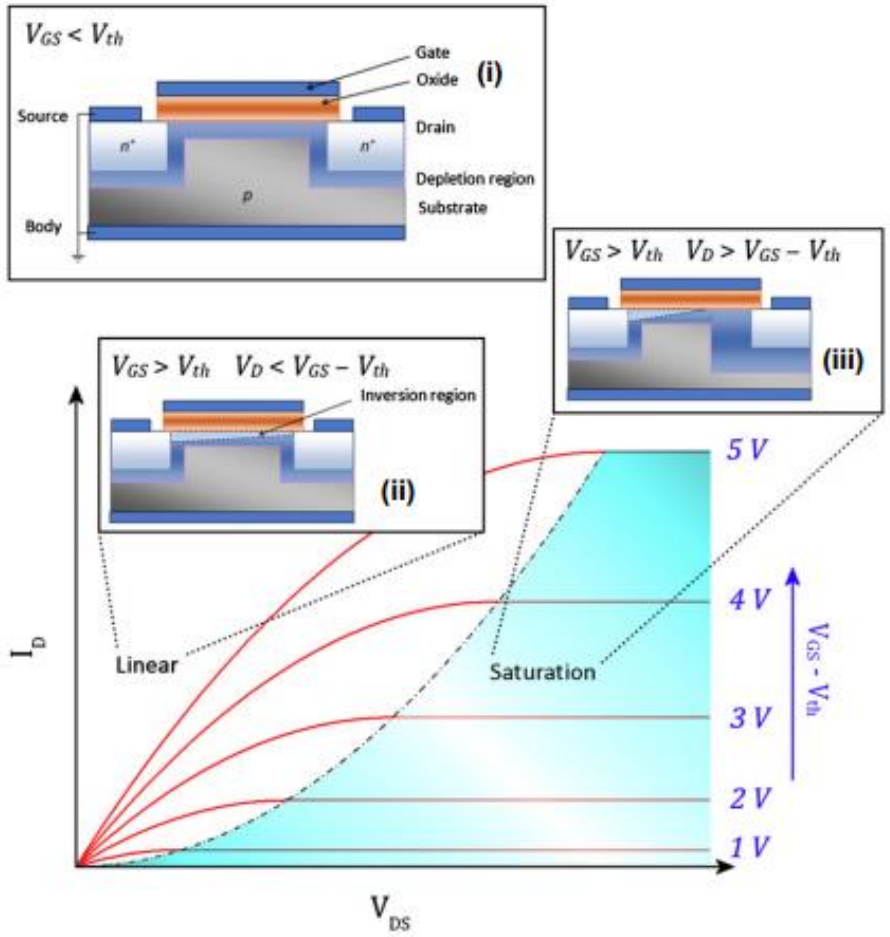
In-silico design of an all-armchair GNRFET sensor for the detection of starch

2. Field effect transistors and graphene

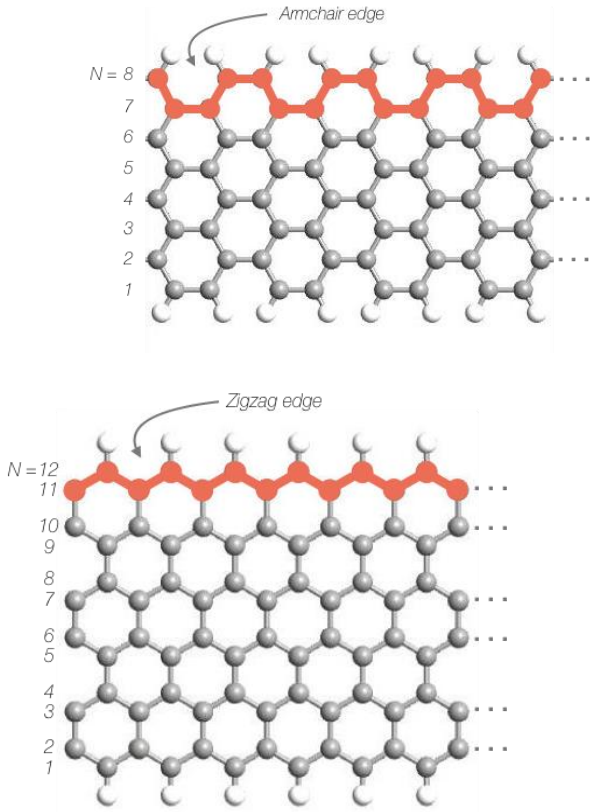


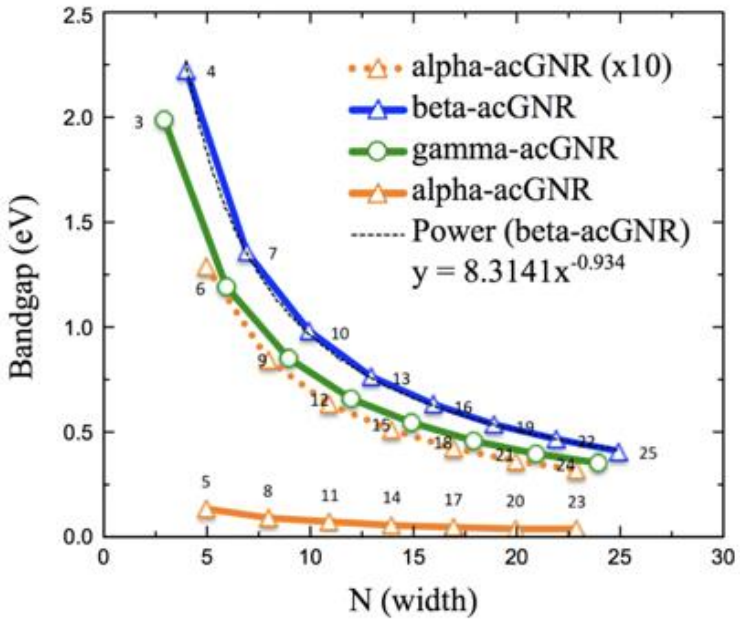
J. H. Warner, F. Schaffel, M. Rummeli, and A. Bachmatiuk,Graphene:Fundamentals and emergent applications.Newnes, 2012, ch. 6.1, pp.333–346.

2. Field effect transistors and graphene



J. H. Warner, F. Schaffel, M. Rummeli, and A. Bachmatiuk,Graphene:Fundamentals and emergent applications.Newnes, 2012, ch. 6.1, pp.333–346.

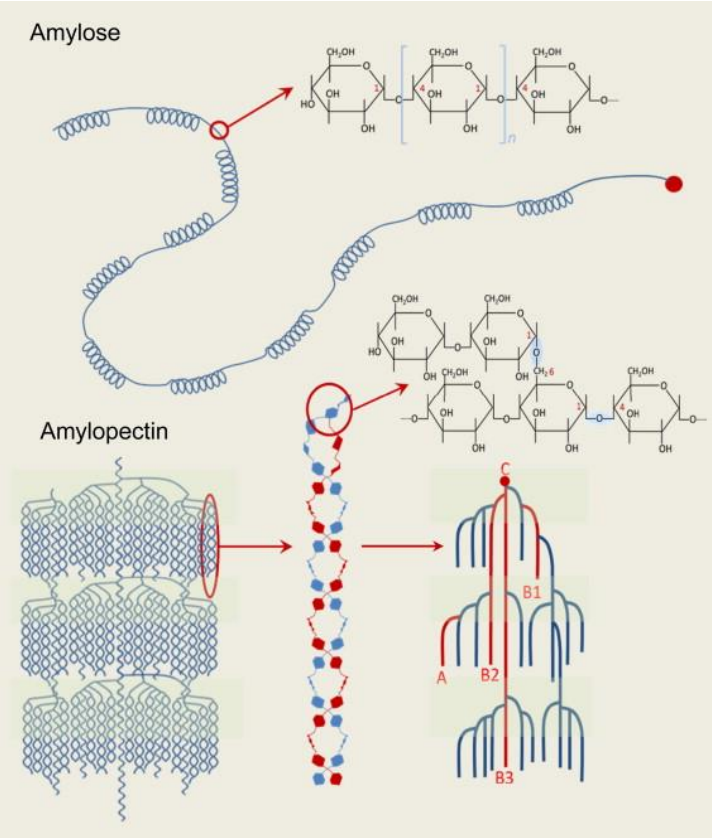




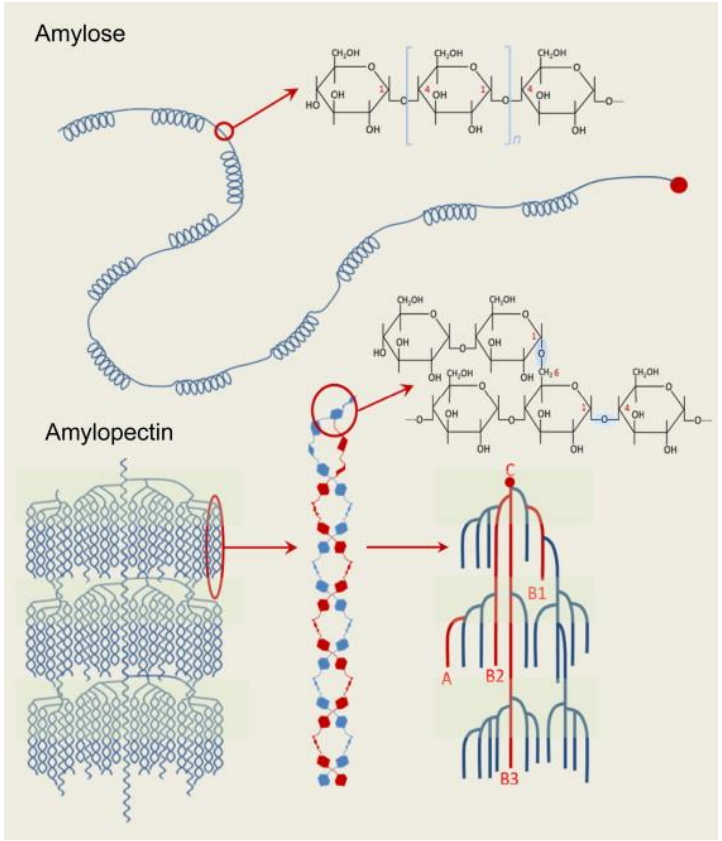
Jaramillo-Botero, A., & Marmolejo-Tejada, J. M. (2019). All-Armchair Graphene Nanoribbon Field-Effect Uridine Diphosphate Glucose Sensor: First-Principles In-Silico Design and Characterization. *IEEE Sensors Journal*, *19*(11), 3975-3983.

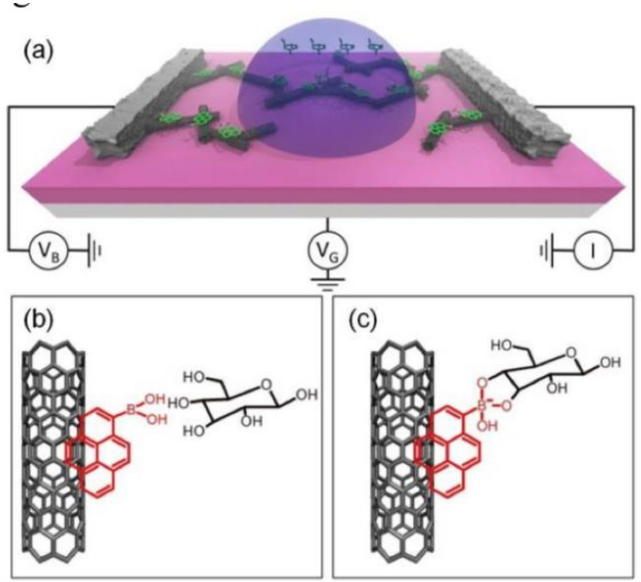
Pontificia Universidad JAVERIANA Cali

3.Design: Functionalization

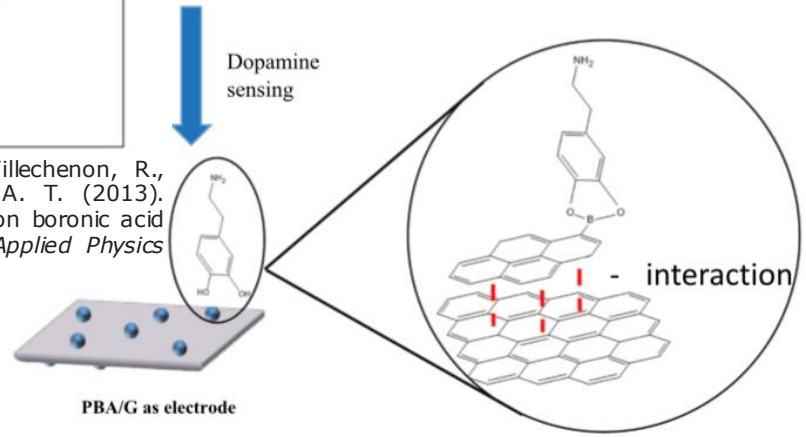


3.Design: Functionalization



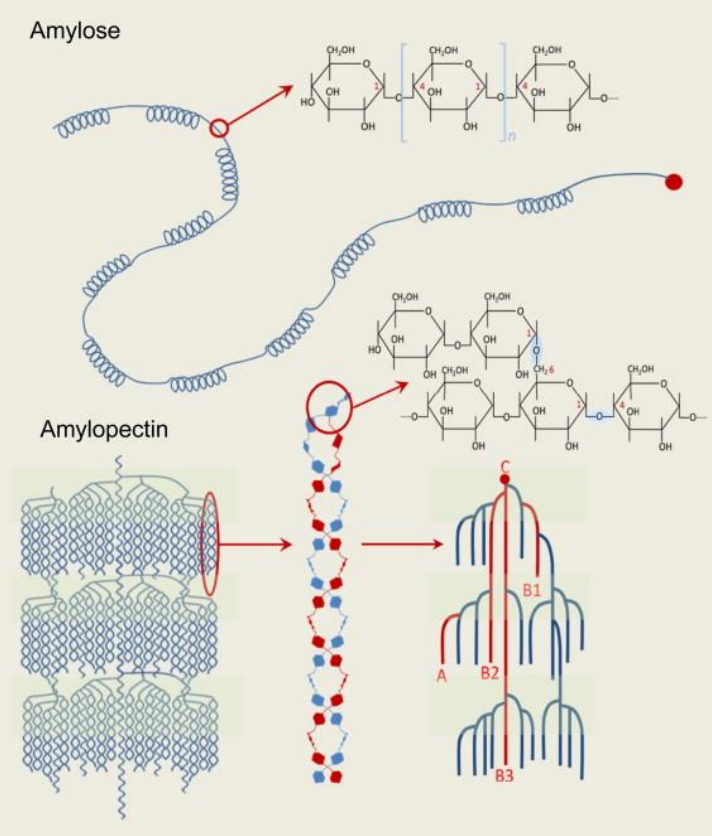


Lerner, M. B., Kybert, N., Mendoza, R., Villechenon, R., Bonilla Lopez, M. A., & Charlie Johnson, A. T. (2013). Scalable, non-invasive glucose sensor based on boronic acid functionalized carbon nanotube transistors. *Applied Physics Letters*, *102*(18), 183113.



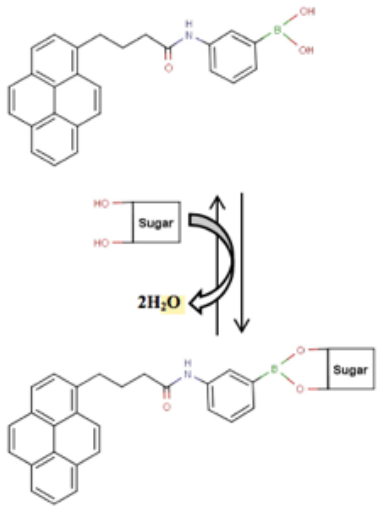
Teo, E. Y. L., Ali, G. A., Algarni, H., Cheewasedtham, W., Rujiralai, T., & Chong, K. F. (2019). One-step production of pyrene-1-boronic acid functionalized graphene for dopamine detection. *Materials Chemistry and Physics*, *231*, 286-291.

3.Design: Functionalization



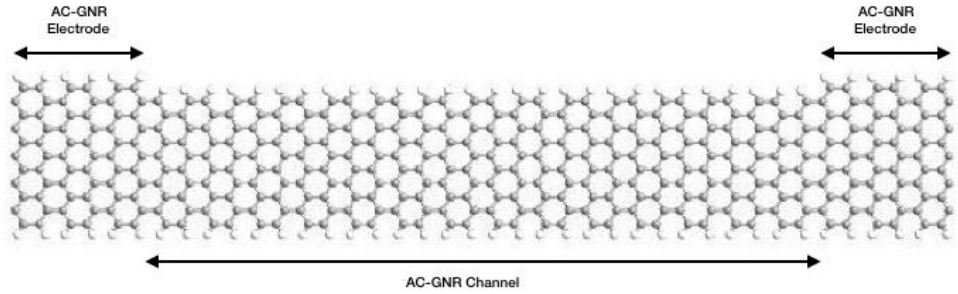
Binding energy (eV)	-0.625766
Binding energy (Kcal/mol)	-14.392618

*Ab-initio calculations using DFT

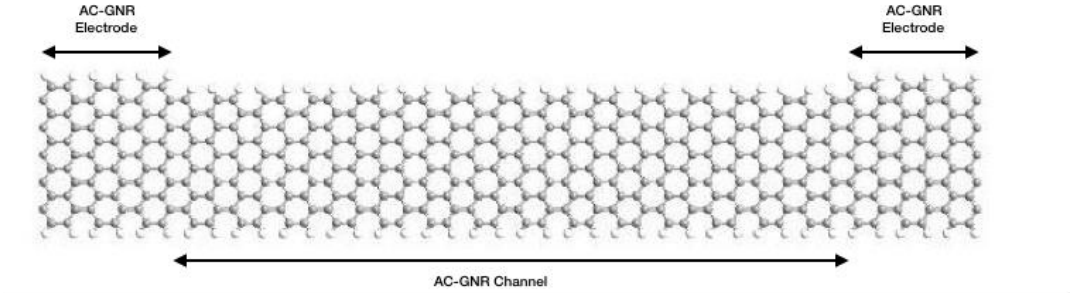


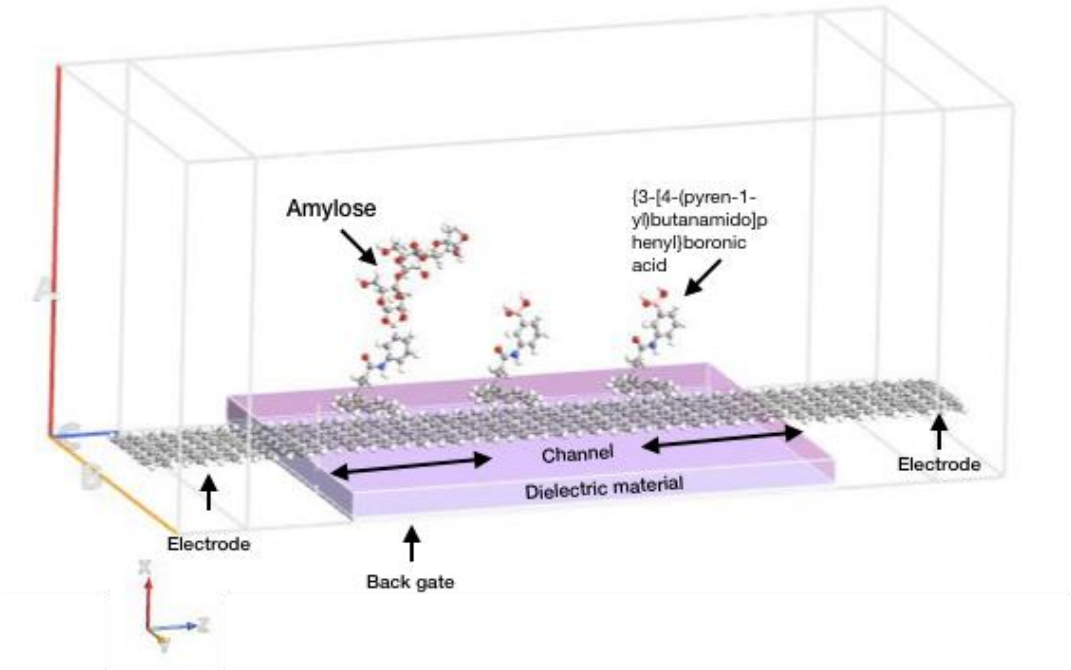
Tlili, C., Badhulika, S., Tran, T. T., Lee, I., & Mulchandani, A. (2014). Affinity chemiresistor sensor for sugars. *Talanta*, *128*, 473-479.

3.Design: Geometry and IV characteristics



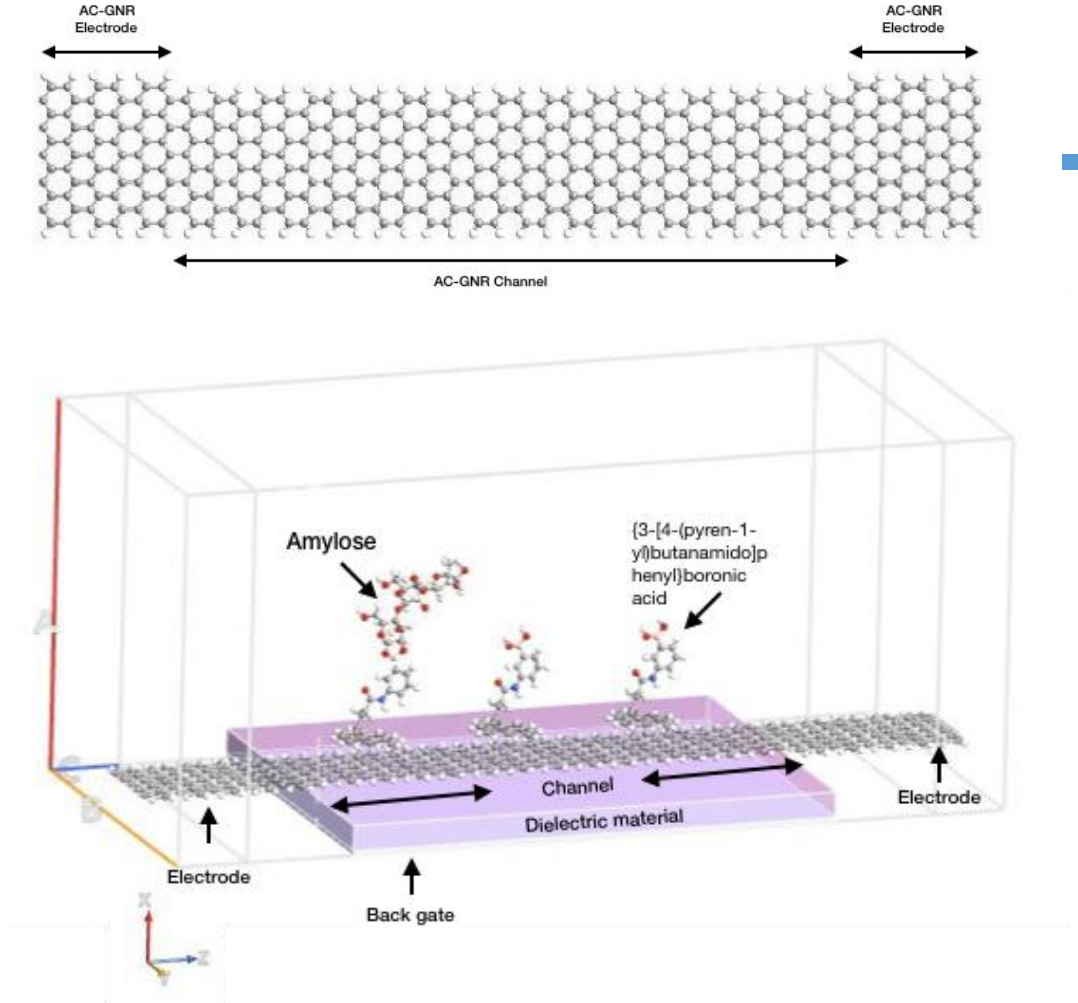
3.Design: Geometry and IV characteristics

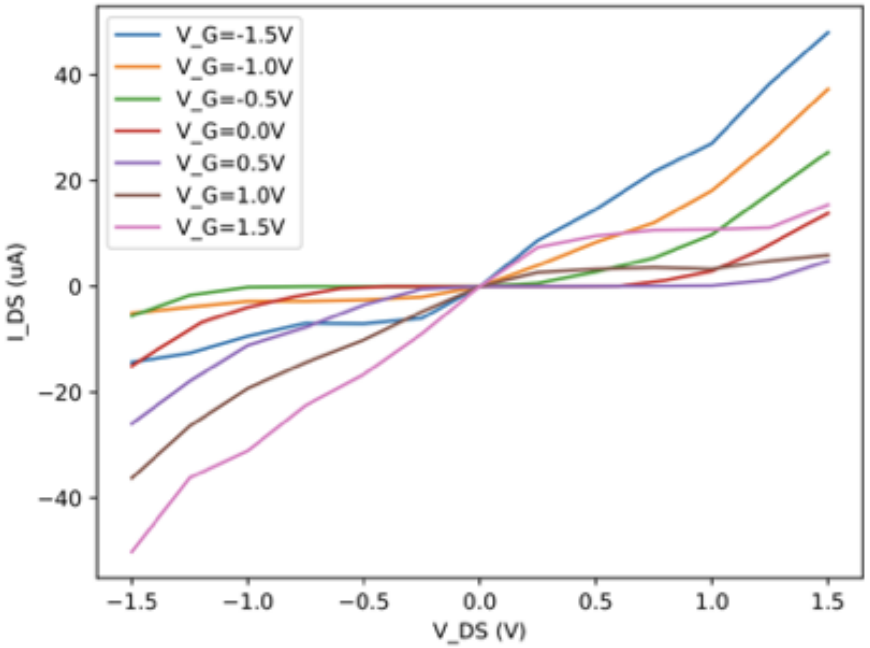




In-silico design of an all-armchair GNRFET sensor for the detection of starch

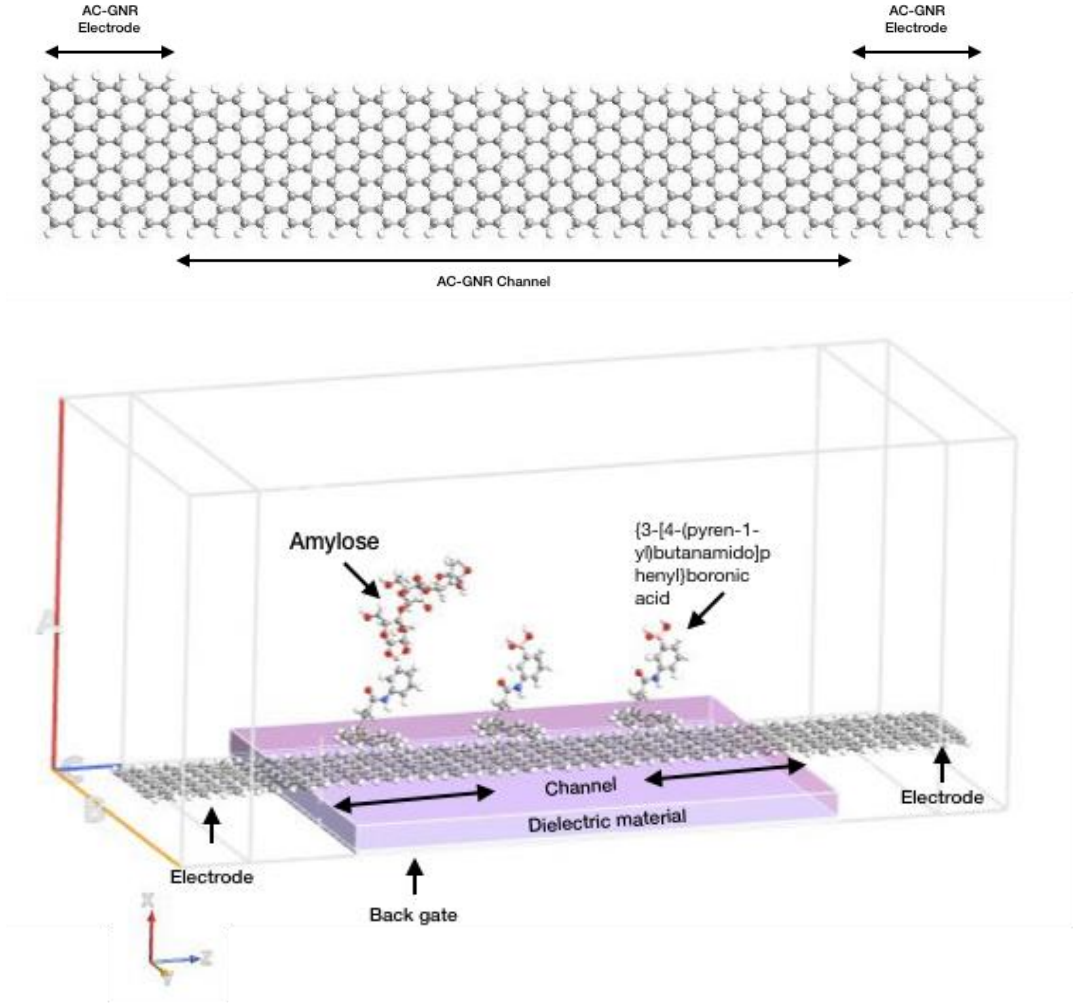
3.Design: Geometry a characteristics

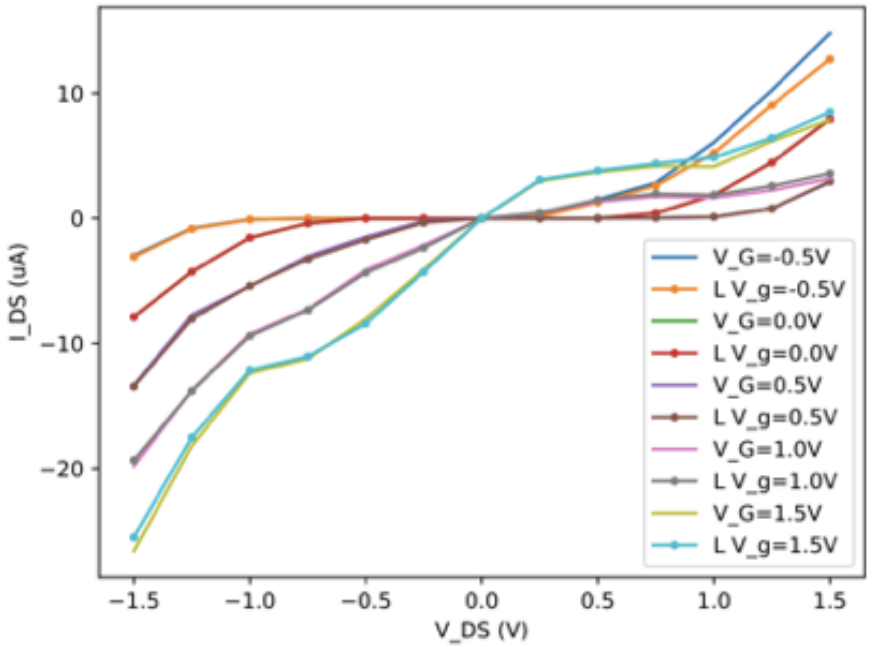




*Calculations using Density Functional Based Tight Binding (DFTB)

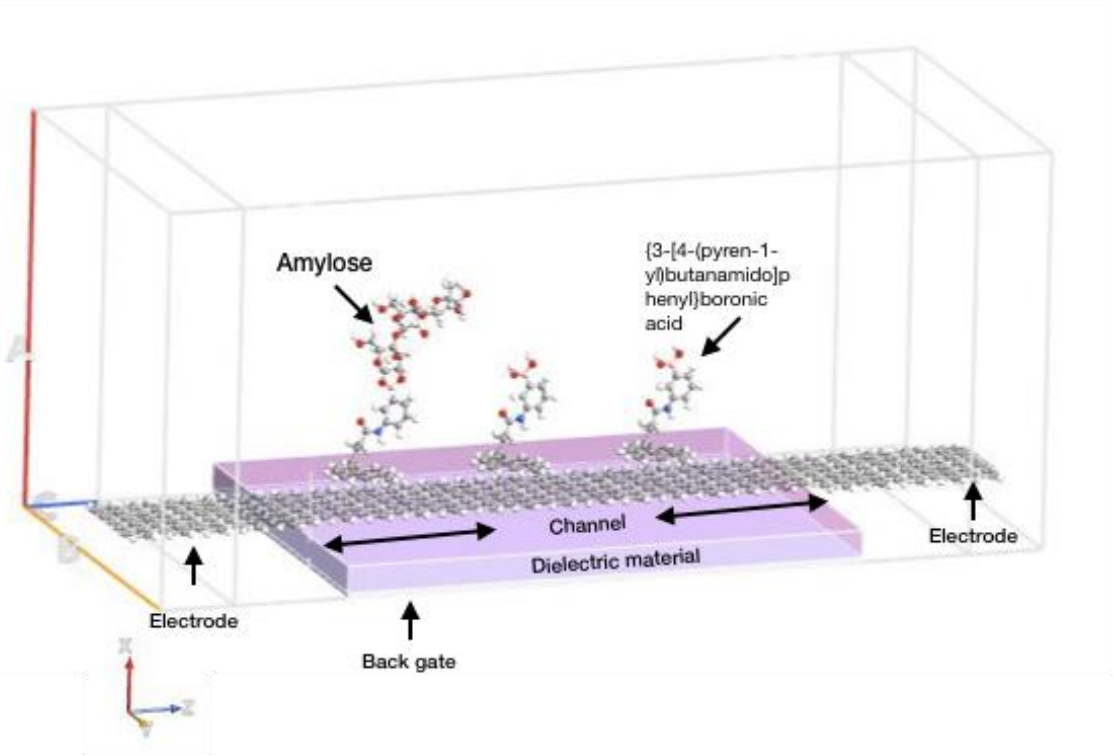
3.Design: Geometry and IV characteristics

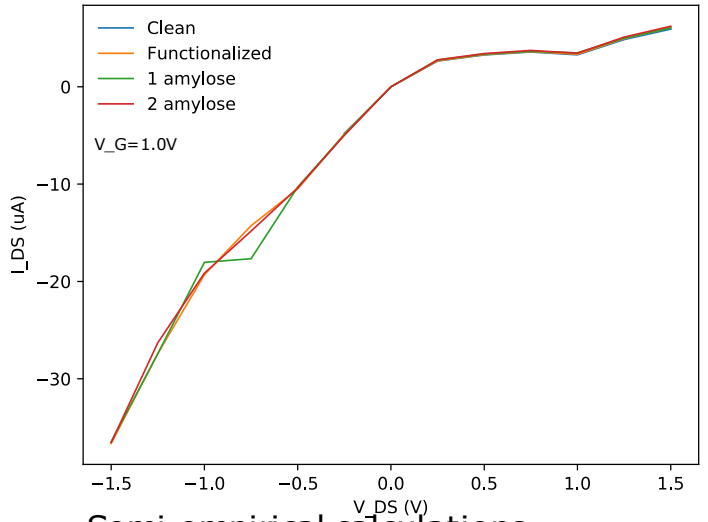




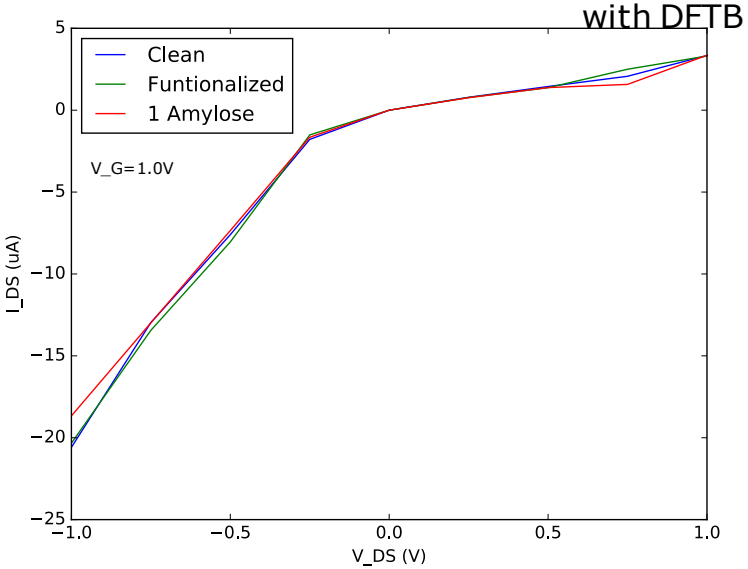
*Calculations using DFTB

3.Design: Geometry and IV characteristics





Semi empirical calculations with DFTB



Ab-initio calculations with Density Functional Theory

4.Conclusions

- Using a single armchair nanoribbon for the electrodes and channel enables a symmetric, compact and practical layout of the transistor
- A graphene-based sensor is a suitable option for this application because:
    - It is an all-carbon highly-biocompatible material
    - The channel provides a high-surface area which is directly exposed to sensing environment