INTRODUCTION

Transition Metal Dichalcogenides (TMDC)

MoS$_2$

Single-layer MoS$_2$ is a semiconductor with a direct band gap of 1.8 eV

Why GO in CMOS devices?
- To add functionality to the device (doping, band alignment control)
- GO fabrication is easier and inexpensive, thanks to solution-processability
- Both GO and MoS$_2$ can be deposited as thin films and are flexible
- It’s possible to have precise control over the number of deposited GO layers

Graphene Oxide (GO)
GO is an insulator composed of a graphene layer with Oxygen functional groups randomly attached on the surface. Oxygen is mainly present as epoxy and hydroxyl functional groups.


RESEARCH PLAN
- Choose an ideal Graphene/MoS$_2$ interface
- Investigate the effect of:
  * Oxygen concentration (max. 25%)
  * Type of Oxygen functional groups (epoxy and hydroxyl, in different ratios)
- Check the distance between GO and MoS$_2$ planes
- Investigate the stability of the interfaces
- DOS and band structure analysis

It has been chosen a 3x3 graphene unit cell and a 4x4 MoS$_2$ one. The distance between S and O has been kept fixed to 2.79 Å. All interfaces are stable.

DEVICE ARCHITECTURES

(a) MoS$_2$ as active layer
- GO between MoS$_2$ and the contacts, to have a p-type FET

(b) MoS$_2$ as conductive channel
- GO as substrate, to have tunable p-doping of MoS$_2$

(c) MoS$_2$ as conductive channel
- GO as gate insulator, as an alternative to HfO$_2$

MAIN RESULTS

- Each point is the average of 10 values
- Error bars indicate the standard deviation of the mean

Reliability check with Hybrid Functional HSE06

With increasing Oxygen concentration in GO, MoS$_2$ becomes increasingly p-doped. This means that GO substrates can be used to:
- tune and control the doping of MoS$_2$
- tune and control the Schottky barrier height (SBH) at the interface

Using a GO with high Oxygen concentration, it is possible to fabricate a p-type CMOS device.
- Epoxy functionalization gives higher SBH compared to hydroxyl one.
- Charge transfer occurs at the interface, with electrons being transferred from MoS$_2$ to GO. This effect is enhanced in presence of higher concentration of oxygen in the GO layer.

With high Oxygen concentration, it is possible to fabricate a p-type CMOS device.

Methods

DFT (VASP code)
- Conjugate-gradient method used to relax the ions to less than 0.03 eV/Å residual atomic forces
- GGA (PBE exchange-correlation functional) and hybrid functional (HSE06)
- Plane-Wave basis set (wave function kinetic energy cutoff of 500 eV)
- PAW method to describe the core electrons
- Gamma-centered 9x9x1 k-points mesh
- Van der Waals included (DFT-D2)
- Spin-orbit interactions not included

Charge transfer analysis (Bader)