MoS$_2$/Graphene Oxide as novel semiconductor/oxide interfaces for electronics

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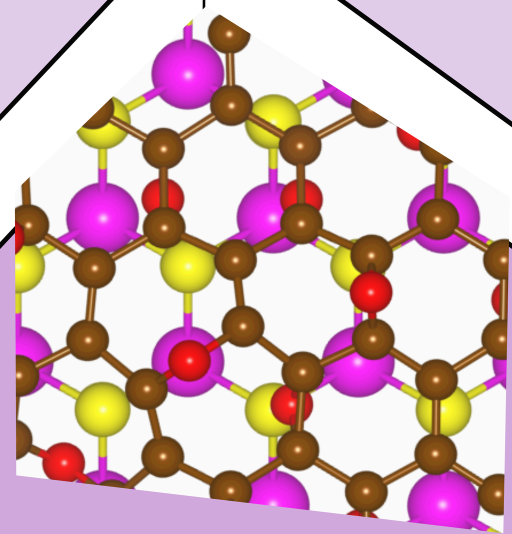
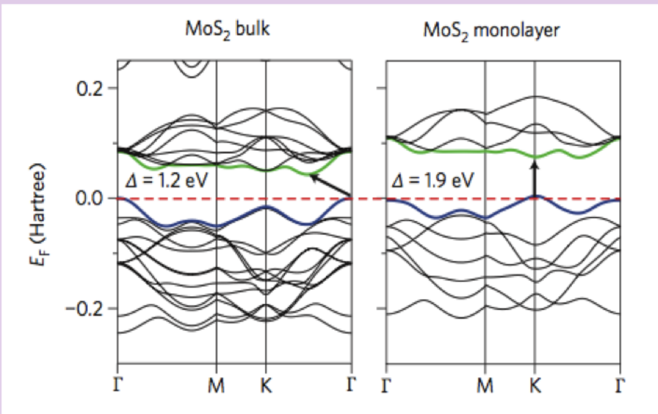


INTRODUCTION

MoS$_2$

Transition Metal Dichalcogenides (TMDC)

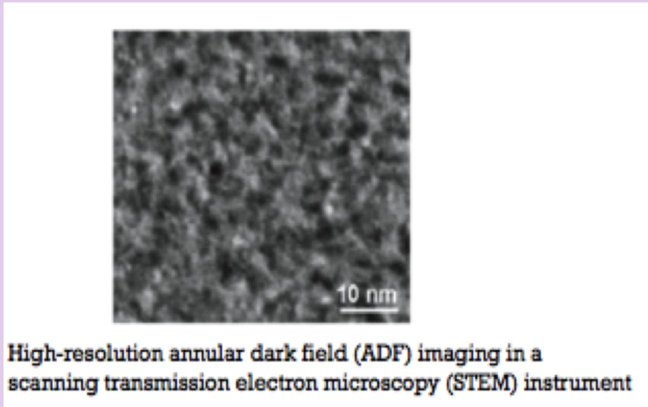
Single-layer MoS$_2$ is a semiconductor with a direct band gap of 1.8 eV



Wang et al, Nature Nanotechnology 7 (11), 2012

Graphene Oxide (GO)

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



High-resolution annular dark field (ADF) imaging in a scanning transmission electron microscopy (STEM) instrument

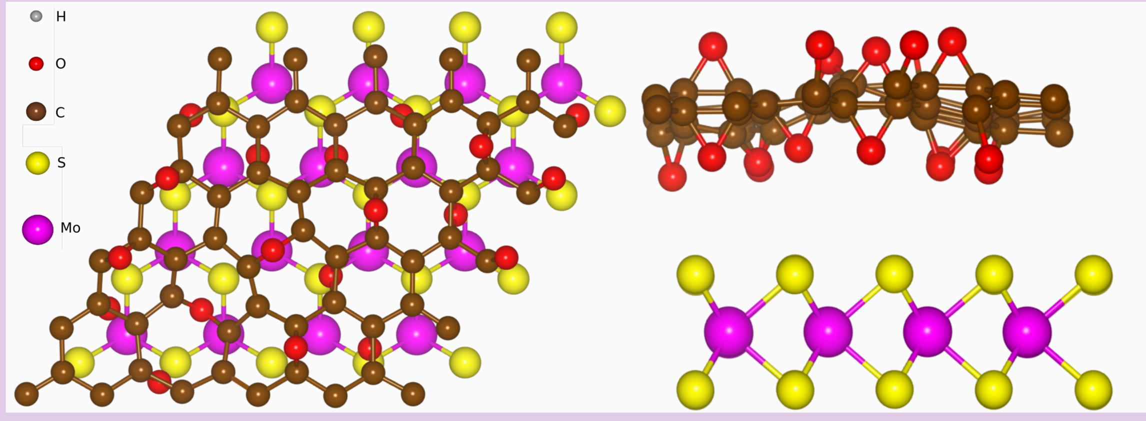
Eda G. and Chowalla M., Advanced Materials 22 (22), 2010

Why GO in CMOS devices?

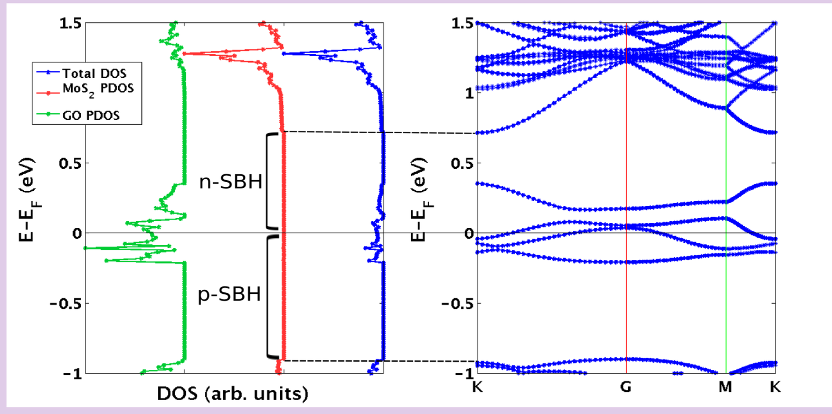
- To add functionality to the device (doping, band alignment control)
- GO fabrication is easier and inexpensive, thanks to solution-precessability
- Both GO and MoS$_2$ can be deposited as thin films and are flexible
- it's possible to have precise control over the number of deposited GO layers

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



Relaxed structure of the interface MoS$_2$/GO. GO has just epoxy functional groups.
The total Oxygen concentration in the graphene plane is 24.24%.

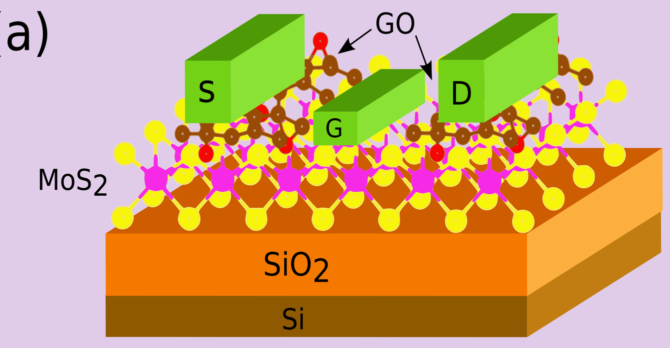


Example of Density of States (DOS) plot with the relative band plot, with definition of n-type and p-type Schottky Barrier Height (SBH).

It has been chosen a (5x5) graphene unit cell and a (4x4) MoS$_2$ one.
The distance between S and O has been kept fixed to 2.79Å.
All interfaces are stable.

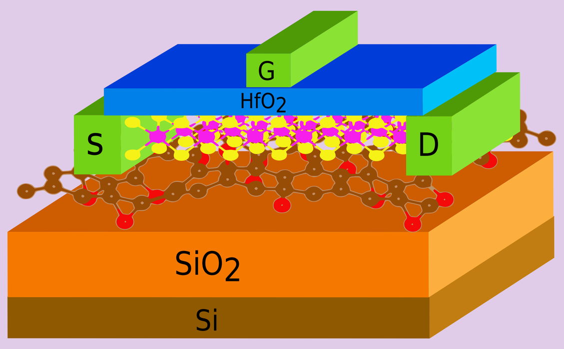
DEVICE ARCHITECTURES

(a)



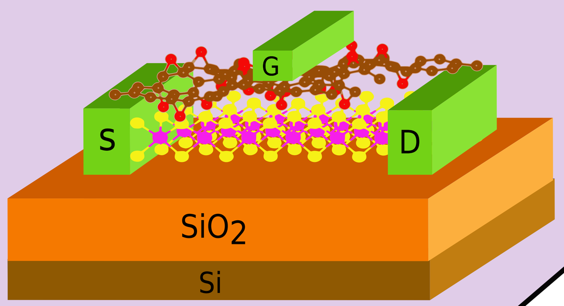
- MoS$_2$ as active layer
- GO between MoS$_2$ and the contacts, to have a p-type FET

(b)



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

(c)

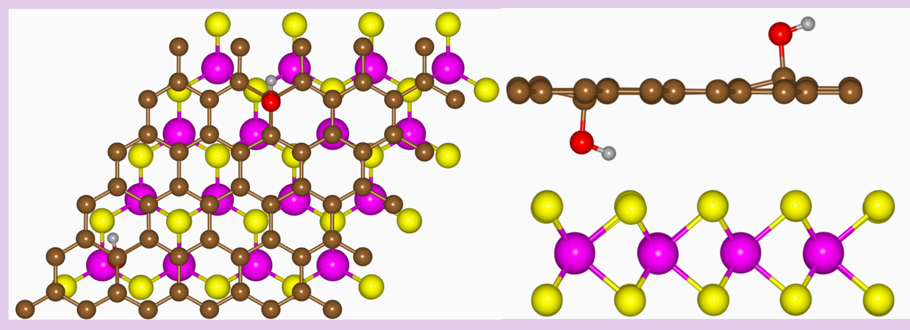


- MoS$_2$ as conductive channel
- GO as gate insulator, as an alternative to HfO$_2$

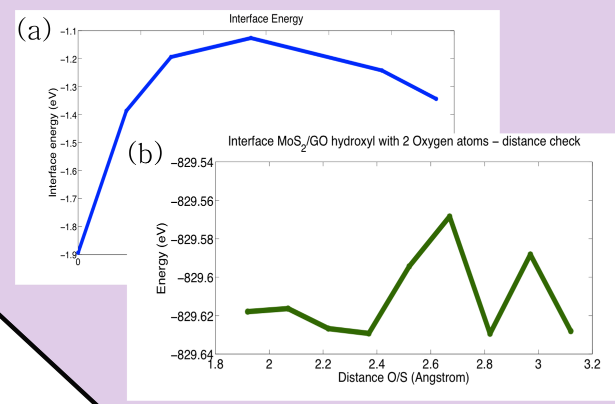
METHODS

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

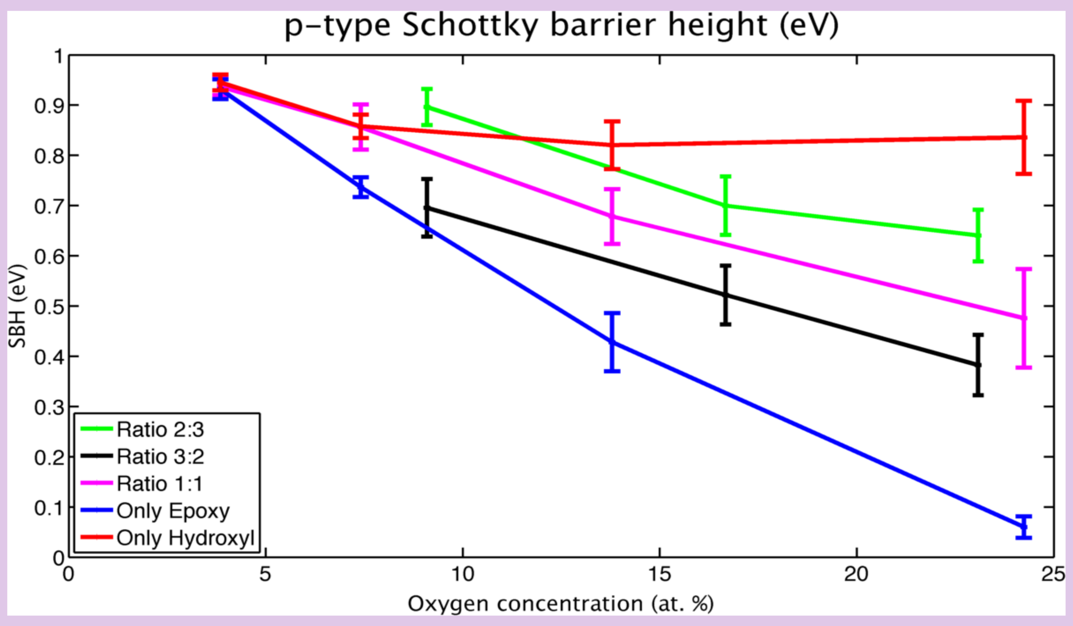


Relaxed structure of the interface MoS$_2$/GO. GO has just hydroxyl functional groups.
The total O concentration in the graphene plane is 3.85 %.



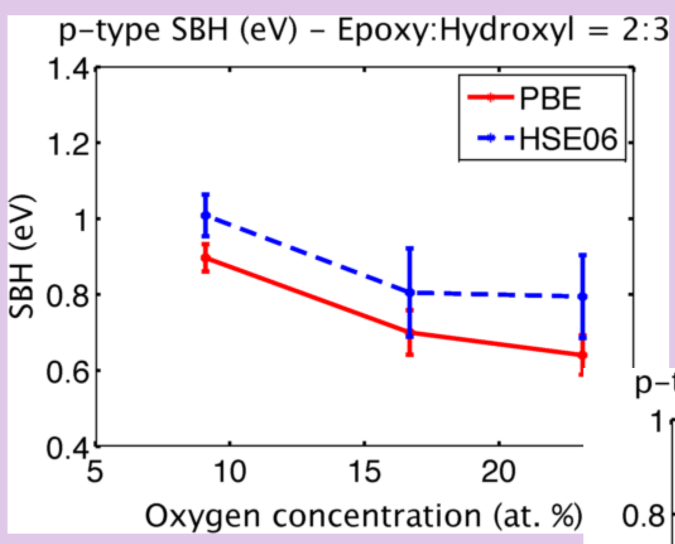
Interface energy in function of Oxygen concentration (a) and energy vs distance between O and S (b) for MoS$_2$/GO interfaces where GO has just hydroxyl functional groups.
The O concentration is 3.85 %.

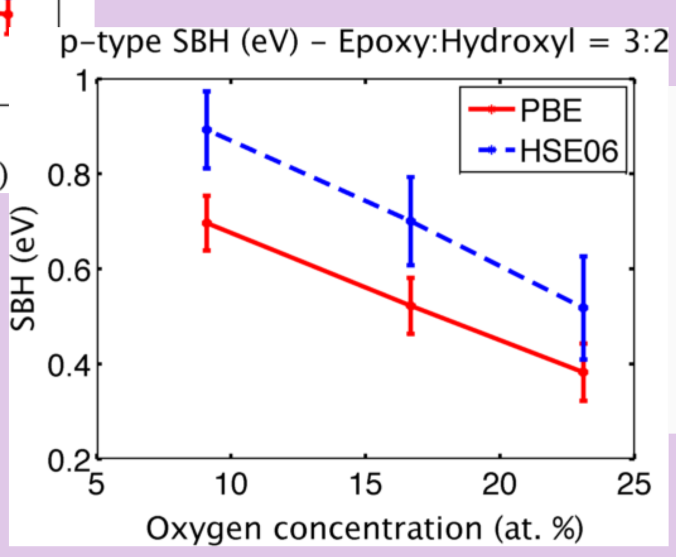
MAIN RESULTS



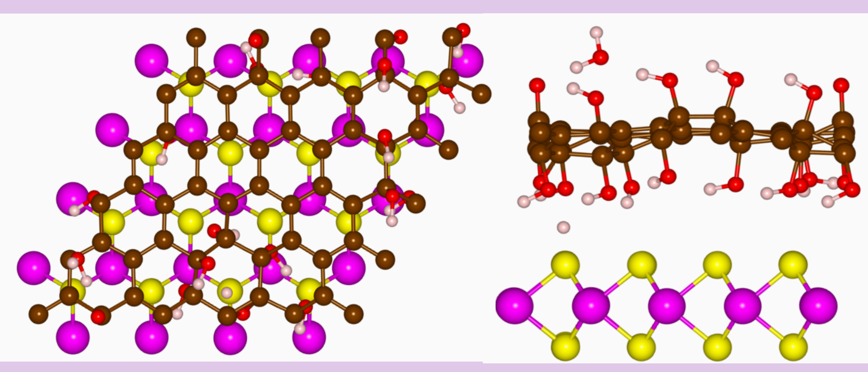
- Each point is the average of 10 values
- Error bars indicate the standard deviation of the mean

- 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.

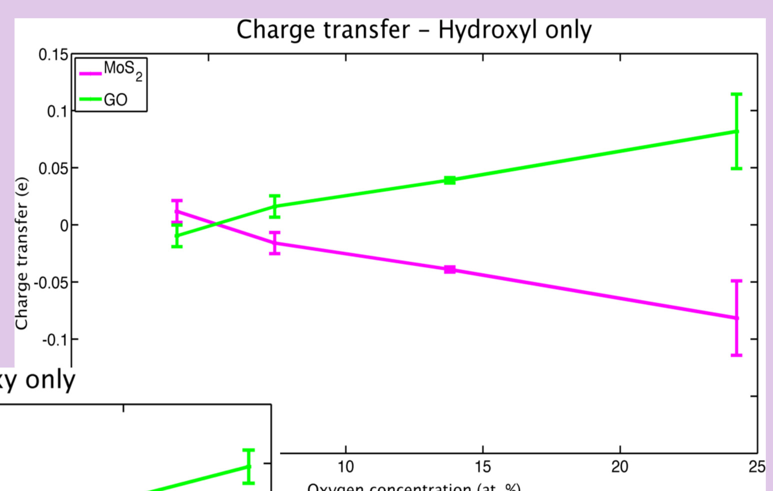


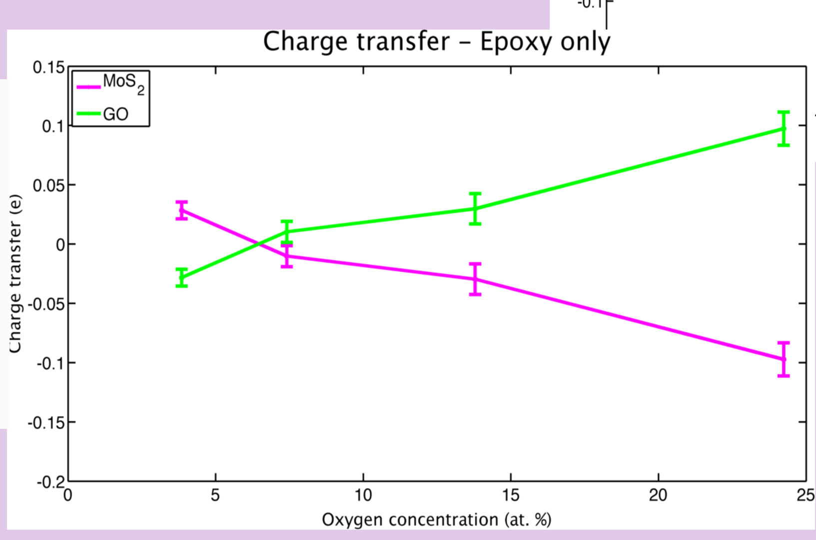


Reliability check with Hybrid Functional HSE06



Relaxed structure of the interface MoS$_2$/GO. GO has just hydroxyl functional groups.
The total Oxygen concentration in the graphene plane is 24.24%.
There is formation of water.





Charge transfer analysis (Bader)