

# Hydrogen Adsorption and Electronic Transport in Graphene Grain Boundaries

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Graphene and other 2D materials have been shown to be enormously sensitive to local disorder and especially line defects or grain boundaries (GB) have turned out to have a significant impact on the electronic structure [1]. Furthermore, investigated line defects have shown altered chemical reactivity allowing researchers to tailor the properties of graphene using chemical functionalization [2].

In this work we have chosen to investigate the 558 GB (Fig. 1) due to its simplicity, symmetry and system size, making it ideal to study with density functional theory.

We have performed plane-wave calculations in order to determine the adsorption barriers of hydrogen atoms near and on the GB. Key sites with low adsorption barriers are then chosen in order to determine the impact of hydrogenation on the electronic transmission across the GB. The latter is calculated using the new and improved TransIESTA package [3].

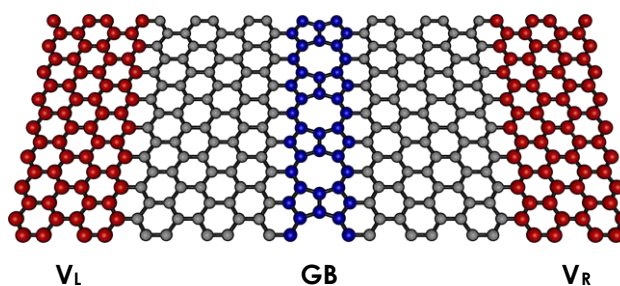
Finally, we have performed transport calculations on the "clean" GB to investigate the impact of gating while applying a bias across the defect from  $V_L$  to  $V_R$ .

We discuss the intricate details of the doping and bias dependence of the GB, as well as the impact of hydrogenation.

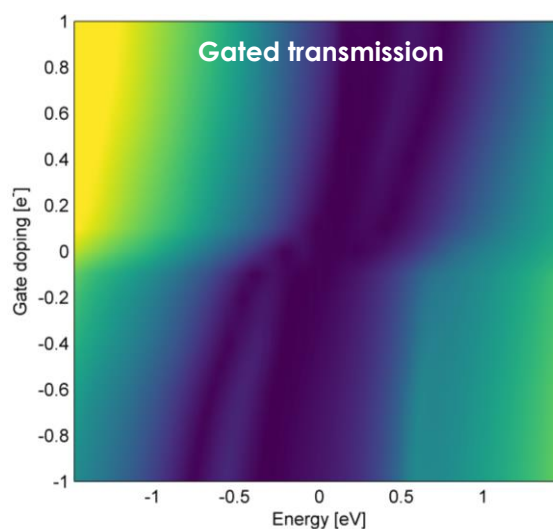
## References

- [1] A. Luican-Mayer *et al.*, "2D Materials", 3.3 (2016) 031005.
- [2] J.-E. Barrios-Vargas *et al.*, "2D Materials", 4.2 (2017) 025009.
- [3] N. Papior *et al.*, "Computer Physics Communications", 212 (2017) 8-24.

## Figures



**Figure 1:** Graphene sheet with a 558 line defect. The grain boundary is highlighted, as well as the electrodes used in our calculations.



**Figure 2:** Contour plot of transmission function calculated at a fixed bias (0.4 V) with varying energy and doping level of the system.