Manipulating the electronic properties of graphene on the SiC(0001) surface via intercalation and molecular adsorption: a first-principles study

Nuala M. Caffrey[1,2]
Rickard Armiento[1], Rositsa Yakimova[1] & Igor A. Abrikosov[1]

[1]*Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden*
[2]*School of Physics & CRANN, Trinity College, Dublin 2, Ireland*

Nuala.Caffrey@tcd.ie

The thermal decomposition of silicon carbide (SiC) is one of the most promising methods to produce high-quality epitaxial graphene on a wafer scale. Sufficient control has even been achieved, on the SiC(0001) face, to selectively grow monolayer, bilayer and few-layer graphene, rendering it a indispensable technique for the future manufacturing of graphene-based electronics.

A disadvantage of this method is that the first carbon layer is covalently bonded to the surface Si atoms, with only subsequent layers displaying the characteristic electronic features of graphene. Several methods have been proposed to electronically decouple this so-called buffer layer, as well as to reduce the high substrate induced doping, including intercalation and chemical doping [1,2,3]. Understanding such chemical functionalisations is a fundamental first step towards engineering the properties of graphene on SiC.

We show how charge neutrality in the graphene layer can be achieved by completely passivating the dangling bonds of the clean SiC surface with nitrogen intercalants. Furthermore, we show that the sensitivity of graphene to atmospheric dopants, such as NO2, depends on its interaction with a substrate, as well as on the number of graphene layers present [4,5].

References

[1] N.M. Caffrey et al., Phys. Rev. B, 92 (2015) 081409
[2] C. Riedl et al., J. Phys. D: Appl. Phys., 43 (2010) 374009
[3] K. V. Emtsev et al., Phys. Rev. B, 84 (2011) 125423
[4] R. Pearce et al., Sensor Actuat B-Chem, 155 (2011) 451; ACS Nano, 7 (2013) 4647
[5] N.M. Caffrey et al., Phys. Rev. B, 94 (2016) 205411

Figures

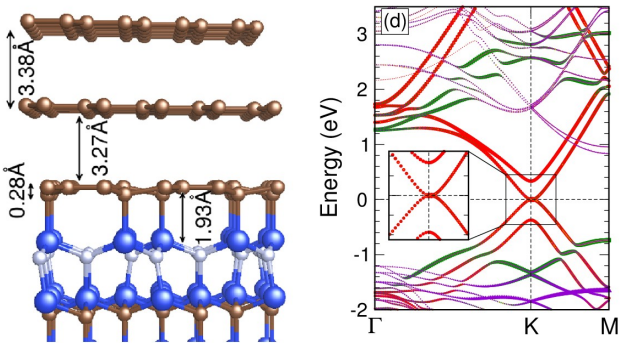

Figure 1: Left: Structure of bilayer graphene on SiC(0001) with an intercalating Si-N layer at the interface. Right: Associated electronic band structure.