A Deep Insight into Defect Engineering at the Metal-Graphene and Metal-Phosphorene Interfaces

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Abstract

Invention of Graphene [1] and other 2D materials is the new hope for the semiconductor device scaling but the contact resistance is the main bottleneck for their performance improvements due to Schottky barrier, tunnel barrier and various trap states. Defect engineering is a promising technique for contact resistance improvement in Graphene based transistors [2] [3], but its physics and the chemistry at the interface need to be explored more. Defect engineering at other 2D elemental material contacts like Phosphorene is also not explored yet.

In this work, we have explored the interface chemistry and carrier transport physics of Graphene and Phosphorene with metal (Pd) using DFT and NEGF methods supported in Quantum ATK package. It is observed that the Carbon (C) vacancy at the interface region enhances 'Pd-C' covalent bond while Phosphorous (P) vacancy does not have a major impact on the bonding at Phosphorene-Pd interface (Figure 1). Graphene has weak vdW interaction with Pd due to unavailability of vacant orbital in the C atom. When a C vacancy is created at the interface, Pd-Graphene bond becomes stronger due to vacant orbitals available at the three nearest neighbour C atoms of the vacant site which reduces bond length from 2.61 Å to 2.50 Å (Figure 1). Phosphorene has relatively stronger bond with Pd due to interaction of Pd electron cloud with vacant 3d orbitals of P. However, unlike Graphene-Pd interface, the bond length is not significantly affected (2.20 Å to 2.18 Å) in the presence of P vacancy at the interface. Reduction in bond length enhances the carrier transmission probability (Figure 2) and hence reduces the contact resistance (~2.3 times) due to reduction in tunnel barrier at the Pd-Graphene interface. P vacancy doesn't result in a significant improvement in contact resistance at Pd-Phosphorene interface due to insignificant changes in the tunnel barrier.

References

[1] K. S. Novoselov et al., Science, 306 (2004), 666–669
[2] Mayur Ghatge et al., IEEE Trans. on Electron Devices, 62, 12 (2015) 4139-4147.
[3] Adil Meersha et al., IEDM (2016)

Figures

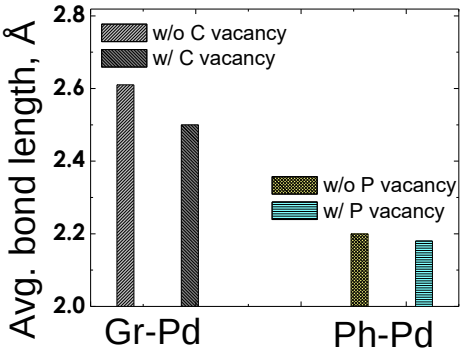

Figure 1: Carbon-Pd and Phosphorous-Pd bond lengths at intrinsic and the defected interfaces.

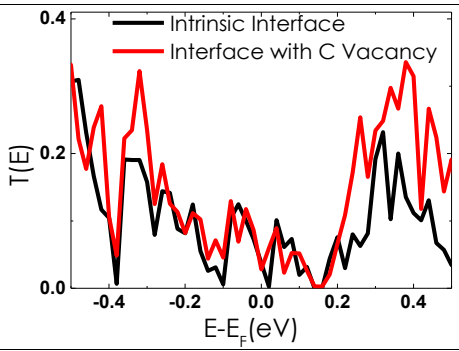

Figure 2: Carrier transmission probability near fermi level (0 eV) for intrinsic and defected Graphene-Pd interfaces. C vacancy enhances the transmission probability near Fermi level.