H coverage defects in quasi free standing graphene

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Quasi free standing graphene (QFSG) on SiC is obtained by intercalating H atoms at the interface between the carbon rich buffer layer obtained by Si evaporation and SiC(0001) substrate. The procedure produces a flat and completely sp^2 hybridized honeycomb lattice [1]. The regularity of this graphene sheet is however interrupted by localised features appearing in the STM images as bright and dark spots, whose brightness depends on the bias voltage. Varying the temperature of measurement and H intercalation, the amount and distribution of spots varies, appearing in some cases located on a lattice with ~6×6 SiC periodicity. These features were attributed to vacancies in the H coverage [2].

In order to clarify the nature of these "spots", we evaluated the structural and electronic properties of quasi free standing graphene with defects in H coverage within the Density Functional Theory (DFT) framework, using a calculation setup previously tested in similar systems [3]. For calculations, we use two kind of supercells: the $6\sqrt{3}\times6\sqrt{3}$ (~1400 atoms) including up to two vacancies per cell, and a smaller one, $\sqrt{31}\times\sqrt{31}$, which includes a slight rotation of graphene with respect to SiC (~0.7 deg), and a single vacancy per cell, but is considerably smaller (~400 atoms). This allowed extensively evaluating and comparing a large number of vacancies with size in the range 1-13 missing H (see Fig 1 for a sample of cases) and with different translations relative to graphene lattice. Calculations show that inward bending is present in correspondence of the vacant sites, whose depth and width increase with the size of the vacancy. A comparison of simulated and measured AFM images indicates that the range of the revealed vacancies is 2-4 missing atoms. The analysis of the electronic structure and DoS reveals localised electronic states between graphene and SiC, with energy and intensity depending on the vacancy size. This allows interpreting the different relative brightness of observed STM features. Besides, the extensive evaluation of the vacancy energies indicates that their stability increases up to the size of ~7 vacant Hs. The most favourable location conformation and location of vacancies with respect to the graphene lattice are also revealed, shedding some light on the H intercalation/evaporation process.

References

[1] Riedl C. et al., PRL, 103 (2009) 246804
[2] Murata Y. et al., APL, 105 (2014) 221604
[3] Cavallucci T., Tozzini V., JPCC, 120 (2016) 7670

Figures

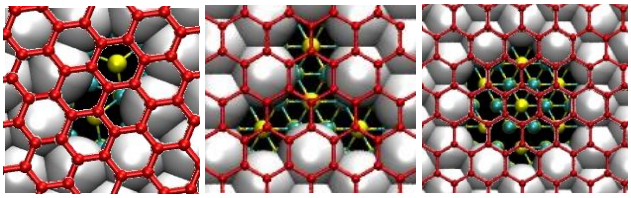

Figure 1: A sample of the studied vacancies in the H intercalation layer. From left to right: 2 missing H, 4 missing H and 7 missing H.