Hydrogen and Graphene: from tuning of hydrogen adsorption by gate voltage, to Si dangling bonds in quasi-free-standing monolayer graphene

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To realize applications of hydrogen-adsorbed graphene, a main issue is how to control hydrogen adsorption/desorption at room temperature. In the first part of the talk, I will demonstrate the possibility to tune hydrogen adsorption on graphene by applying a gate voltage [1]. The influence of the gate voltage on graphene and its hydrogen adsorption properties was investigated by electrical transport measurements, scanning tunneling microscopy (STM), and density functional theory (DFT) calculations. We show that more hydrogen adsorbs on graphene with negative gate voltage (p-type doping), compared to that without gate voltage or positive gate voltage (n-type doping). Theoretical calculations explain the gate voltage dependence of hydrogen adsorption as modifications of the adsorption energy and diffusion barrier of hydrogen on graphene by charge doping.

Si dangling bonds at the interface of quasi-free-standing monolayer graphene (QFMLG) are known to act as scattering centers that can severely affect carrier mobility. In the second part of the talk, I will discuss the atomic and electronic structure of Si dangling bonds in QFMLG using low-temperature STM, spectroscopy (STS), and atomic force microscopy (AFM) investigations together with DFT calculations [2]. Two types of defects with different contrast were observed on flat graphene terraces by STM and AFM; in particular, their STM contrast varied with bias voltage. Moreover, these defects show characteristic STS peaks at different energies, 1.1 and 1.4 eV. The comparison of the experimental data with the DFT calculations indicates that the defects with STS peak energies of 1.1 and 1.4 eV consist of clusters of three and four Si dangling bonds, respectively. The relevance of the present results for the optimization of graphene synthesis is discussed.

[1] Yuya Murata, Arrigo Calzolari, and Stefan Heun, J. Phys. Chem. C 122, 11591 (2018).

[2] Yuya Murata, Tommaso Cavallucci, Valentina Tozzini, Niko Pavliček, Leo Gross, Gerhard Meyer, Makoto Takamura, Hiroki Hibino, Fabio Beltram, and Stefan Heun, Nano Research 11, 864 (2018).