Atomic and electronic structure of Si dangling bonds in quasi-free-standing monolayer graphene

Yuya Murata,[1] Tommaso Cavallucci,[1] Valentina Tozzini,[1] Niko Pavliček,[2] Leo Gross,[2] Gerhard Meyer,[2] Makoto Takamura,[3] Hiroki Hibino,[3] Fabio Beltram,[1] and Stefan Heun[1]

[1]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza San Silvestro 12, 56127 Pisa, Italy
[2]IBM Research-Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland
[3]NTT Basic Research Laboratories, 3-1 Morinosato Wakamiya, Atsugi, Kanagawa 243-0198, Japan

Abstract
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. Herein, we investigate the atomic and electronic structure of Si dangling bonds in QFMLG using scanning tunneling microscopy/spectroscopy (STM/STS), atomic force microscopy (AFM), and density functional theory (DFT) calculations. Two types of defects with different contrast were observed on a flat graphene terrace by STM and AFM; in particular, their STM contrast varied with the bias voltage. Moreover, these defects showed 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.

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(2) Y. Murata, T. Cavallucci, V. Tozzini, N. Pavliček, L. Gross, G. Meyer, M. Takamura, H. Hibino, F. Beltram, and S. Heun, "Atomic and electronic structure of Si dangling bonds in quasi-free-standing monolayer graphene", Nano Res. accepted, DOI: 10.1007/s12274-017-1697-x.