De-Liang Bao

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Fabrication of Millimeter-Scale, Single-Crystal One-Third-Hydrogenated Graphene with Anisotropic Electronic Properties

Periodically hydrogenated graphene is predicted to form new kinds of crystalline 2D materials such as graphane, graphone, and 2D C_xH_y, which exhibit unique electronic properties. Controlled synthesis of periodically hydrogenated graphene is needed for fundamental research and possible electronic applications. Only small patches of such materials have been grown so far, while the experimental fabrication of large-scale, periodically hydrogenated graphene has remained challenging. In the present work, large-scale, periodically hydrogenated graphene is fabricated on Ru(0001). The as-fabricated hydrogenated graphene is highly ordered, with a $\sqrt{3} \times \sqrt{3}/R30°$ period relative to the pristine graphene. As the ratio of hydrogen and carbon is 1:3, the periodically hydrogenated graphene is named "one-third-hydrogenated graphene" (OTHG). The area of OTHG is up to 16 mm^2. Density functional theory calculations demonstrate that the OTHG has two deformed Dirac cones along one high-symmetry direction and a finite energy gap along the other directions at the Fermi energy, indicating strong anisotropic electrical properties. An efficient method is thus provided to produce large-scale crystalline functionalized graphene with specially desired properties.

References

[1] Hui Chen, De-Liang Bao, Dongfei Wang, Yande Que, Wende Xiao, Guojian Qian, Hui Guo, Jiatao Sun, Yu-Yang Zhang, Shixuan Du, Sokrates T. Pantelides, and Hong-Jun Gao, Adv. Mater., 30 (2018) 1801838.

Figures

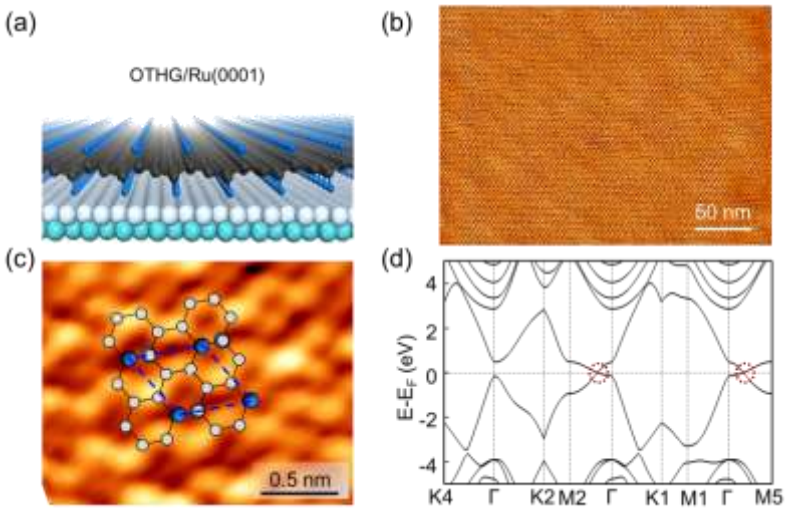

Figure 1: (a) Schematic showing the fabrication of periodically hydrogenated graphene on Ru(0001) through atomic hydrogen chemisorption. (b) A large-scale STM image of OTHG on Ru(0001), showing the formation of hexagonal patters (Sample bias: U = −20 mV, Tunneling current: I = 0.2 nA). (c) Zoom-in STM image of the OTHG (U = −2.0 mV; I = 1.0 nA). The atomic model is superimposed on the STM image. (d) Calculated band structure of the OTHG, using the HSE06 hybrid functional method, showing anisotropic electronic properties. The two Dirac cones at E_F along two high-symmetry paths are indicated with red dashed rings.