

Efficient n -type Doping in Epitaxial Graphene through Strong Lateral Orbital Coupling of Ti Adsorbate

Jih-Wei Chen¹ Camilla Coletti², Stefan Heun³, Chao-Hao Chen⁴, and Chung-Lin Wu¹

¹Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

²Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Pisa 56127, Italy

³NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, 56127 Pisa, Italy

⁴National Synchrotron Radiation Research Center (NSRRC), Hsinchu 30076, Taiwan

paul005paul005@gmail.com

Abstract

Recently, many different types of doping methods for epitaxial graphene have been demonstrated through atom substitution and adsorption. Then, here we observe by angle-resolved photoemission spectroscopy (ARPES) a coupling-induced Dirac cone renormalization when depositing small amounts of Ti onto epitaxial graphene on SiC. We obtain a remarkably high doping efficiency and a readily tunable carrier velocity simply by changing the amount of deposited Ti. First-principles theoretical calculations show that a strong lateral (non-vertical) orbital coupling leads to an efficient doping of graphene by hybridizing the $2p_z$ orbital of graphene and the $3d$ orbitals of the Ti adsorbate, which attached on graphene without creating any trap/scattering states. This Ti-induced hybridization is adsorbate-specific and has major consequences for efficient doping as well as applications towards adsorbate-induced modification of carrier transport in graphene.

Keywords - Graphene, lateral coupling, titanium, angle-resolved photoemission spectroscopy (ARPES), density-functional theory (DFT)