北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Weekly Seminar

Functionalizing Graphene by Intercalations

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Time: 4:00pm, Oct. 28, 2020 (Wednesday)

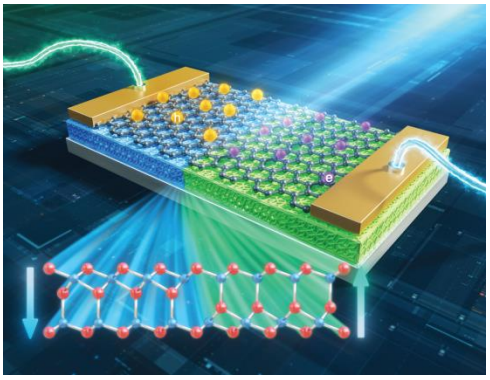
时间: 2020年10月28日 （周三）下午4:00

Venue: Room W563, Physics building, Peking University

地点: 北京大学物理楼，西563会议室

Abstract

The epitaxial growth of graphene on transition-metal substrates has proved to be an efficient method to synthesize high-quality large-area graphene. However, due to the interaction between graphene and the transition-metal substrate, the electronic structure of the as-fabricated graphene is distorted. Intercalating extra materials between graphene and substrates is a way to decouple the interaction between graphene and the substrate and further functionalize graphene. In this talk, combing density functional theory calculations and scanning tunneling microscope experiments, I will show you that the intercalation of traditional two-dimensional semiconducting materials significantly reduces the interaction between graphene and the transition-metal substrate [1]. Multilayer silicene can be intercalated between graphene and Ru(0001) surfaces and form a graphene/silicene van der Waals heterostructure, which shows rectification behavior [2]. It is also found that the intercalated silicon can be oxidized to SiO_2 in both crystalline and amorphous form. The insulating nature of SiO_2 opens new opportunities of the direct synthesis of large scale, device-quality graphene on designed dielectric substrates [3]. We also propose the possible integration of graphene with two-dimensional ferroelectric materials. We find that the intercalated quintuple layer Al_2O_3 or Y_2O_3 is a functional tunnel barrier. Alternating the polarization of intercalated materials modulates the doping type of graphene, enabling the fabrication of graphene p–n junctions [4].



References

[1] Y. Gao, Y.-Y. Zhang, and S. Du, Recovery of the Dirac states of graphene by intercalating two-dimensional traditional semiconductors, *Journal of Physics: Condensed Matter*, **31**, 194001 (2019)

[2] G. Li *et al.*, Stable silicene in graphene/silicene van der Waals heterostructures, *Advanced Materials*, **30**, 1804650 (2018)

[3] H. Guo et al., Insulating SiO_2 under centimeter-scale, single-crystal graphene enables electronic-device fabrication, in revision

[4] X. Jin, Y.-Y. Zhang, S. T. Pantelides, and S. Du, Integration of graphene and two-dimensional ferroelectrics: properties and related functional devices, *Nanoscale Horizons*, **5**, 1303 (2020)

About the speaker

Dr. Zhang, Yu-Yang obtained his PhD in Physics in 2011 at Institute of Physics, Chinese Academy of Sciences, China. He took two terms of postdoc in Rensselaer Polytechnic Institute (with Prof. Shengbai Zhang) and Vanderbilt University (with Prof. Sokrates T. Pantelides). From June 2013 to January 2015, he worked as a guest scientist in Oak Ridge National Laboratory, US. In December 2016, he joined School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China, as an associate professor. His research interest is to use quantum-mechanical calculations based on density functional theory (DFT) to understand the fundamental physics in emerging quantum materials for future nano-electronics, quantum information, and energy-related applications. With such understandings, he designs novel quantum materials, understands the structure-properties correlations, and proposes methods to achieve property modulations for practical applications. His previous and current research projects include first-principle calculations of solid-state materials ranging from crystals, surfaces, interfaces, to various nanostructures. In particular, he studies physics and chemistry at surfaces and interfaces, emergent quantum phenomena, and machine learning in condensed matter physics. More information about Dr. Zhang and his group can be found at www.zhangyuyang.cn