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Gunn Kim

Department of Physics & Astronomy and Graphene Research Institute, Sejong University Republic of Korea

Electronic structures of van der Waals graphene/periodically porous graphene heterostructures

The discovery of graphene has significantly increased research on various two-dimensional (2D) materials such as hexagonal boron nitride and transition-metal dichalcogenides, and the field of 2D materials is expanding to investigate heterostructures containing multiple 2D materials. Recently, several van der Waals heterostructures were prepared experimentally, and the heterostructured materials were found to have unique properties. Consequently, the need for theoretical research to discover and understand the properties of experimentally observed heterostructures has increased. In 2009, a polyphenylene super honeycomb network (PSN) was synthesized, which is a periodic porous graphene sheet with a periodicity of 1 nm or less. Regular, uniform, and porous structures are necessary to increase the performance and expand the applicability of porous carbon materials, including porous graphene. In this talk, I report a first-principle study of the structural and electronic characteristics of vertical graphene/PSN (Gr/PSN) heterostructures. Like vertical graphene/hexagonal boron nitride heterostructures, the vertical Gr/PSN heterostructures also exhibit asymmetry in interlayer potential because PSN is a type of periodic porous graphene sheet. Such interlayer potential asymmetry causes band gap opening in graphene, which may improve the room-temperature pinch-off characteristics of graphene-based field effect transistors. In particular, we focus on the changes in the electronic structure of graphene caused by interactions with PSN. We consider three different stacking configurations for a heterostructure consisting of a graphene sheet and a PSN: AB, AA, and AA'. Regarding the band gap size, we find that a band gap in graphene is induced by stacking with a PSN layer. Besides, we show computationally simulated scanning tunneling microscopy images of the heterostructures. The images show the changes in the electronic structure of a PSN (graphene) layer caused by that of a graphene (PSN) layer on each surface, as well as the pore shapes exhibited on each side of the heterostructure for the stacking configurations.

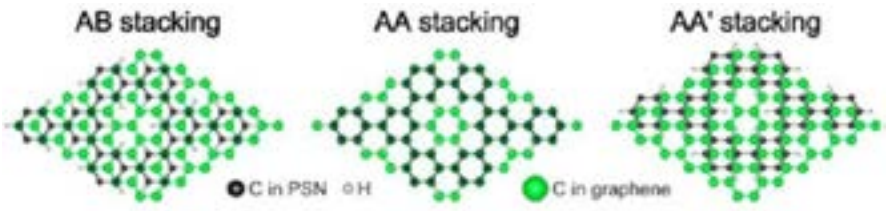

Figure 1: Ball-and-stick model structures of three different stacking types of van der Waals heterostructures

Recent Publications

1. Lee J and Kim G (2017) Electronic properties of a graphene/periodic porous graphene heterostructure. Carbon 122:281-286.
2. Shehzad M A, Hussain S, Lee J, Jung J, Lee N, Kim G and Seo Y (2017) Study of grains and boundaries of molybdenum diselenide and tungsten diselenide using liquid crystal. Nano Letters 17:1474-1481.
3. Lee Y, Kim G and Kwon Y K (2017) *Ab initio* study of aspirin adsorption on single-walled carbon nanotubes. Physical Chemistry Chemical Physics 19:8076-8081.

4. Lee J, Kim M, Chelikowsky J R and Kim G (2016) Computational simulation of subatomic AFM and STM images for graphene/hexagonal boron nitride heterostructures with intercalated defects. Physical Review B 94:035447.
5. Park C, Ryou J, Hong S, Sumpter B G, Kim G and Yoon M (2015) Electronic properties of bilayer graphene strongly coupled to interlayer stacking and an external electric field. Physical Review Letters 115:015502.

Biography

Gunn Kim is an Associate Professor of Theoretical Condensed Matter Physics at Sejong University in Republic of Korea. He has his expertise in computational simulations to investigate physical and chemical properties of various nanomaterials using density functional theory. Recently, he has focused on studying the geometrical and electronic characteristics of the van der Waals heterostructures consisting of two-dimensional nanomaterials such as graphene, hexagonal boron nitride, and transition metal dichalcogenides etc., in terms of defect engineering. All the research topics will lead to better understanding of fundamental issues in the behavior of nanomaterials or to solutions for practical problems in electronic and biological applications.

gunnkim@sejong.ac.kr

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