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Atomic-scale study of lateral graphene/h-BN hybrid structure[1]

JAEKWANG LEE, JEWOOK PARK, AN-PING LI, MINA YOON, Oak Ridge National Laboratory — Recently, atomically sharp 1D interfaces have been successfully implemented in lateral graphene/hexagonal boron nitride (h-BN) hybrid structures. Graphene/h-BN interfaces are of particular interest, because their bandgap and magnetic properties can be engineered by controlling the arrangement of nonmagnetic B, C and N atoms. Despite the enormous interest in graphene/h-BN, there has been very limited experimental success in determining the local atomic structure of the graphene/h-BN interface. Here, using state-of-the-art scanning tunneling microscopy, we report the direct and precise observation of a graphene/h-BN interface bonding structure at the atomic scale. Based on the detailed atomic structure, first-principles density-functional calculations show that graphene zigzag edge states and the h-BN polarity are strongly coupled to each other near the interface and induce spatial modulation of physical properties along the lateral direction. In addition, we investigate how the d-orbitals of metal surfaces (Cu (111), Cu (001)) and the pi-orbital of graphene/h-BN hybridize and predict resulting modification of the electronic properties of graphene/h-BN.

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Jaekwang Lee
Oak Ridge National Laboratory

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