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Electric-field-dependent electronic structure of graphene bilayer: from the Bernal stacking to the unconventional orthorhombic stacking
GUNN KIM, Sejong University, CHANGWON PARK, MINA YOON, Oak Ridge National Laboratory — In this presentation, we report the electronic properties of bilayer graphene structures with various stackings, which can be formed, for instance, during the structural transition from graphite-to-diamond at high pressure, or at boundaries of stacking domains or at diamond surfaces. We performed ab initio calculations and the Wannier interpolations for accurate two-dimensional band structure with extremely dense (1600×1600) k -point grid. Using tight-binding parameters obtained from maximally localized Wannier function analysis, we also constructed the effective Hamiltonian for the graphene bilayer with various stacking. The overall electronic structures can be described by the relative shift and the coupling of two Dirac cones, depending on their stacking geometry. Our results reveal that external electric field is another parameter to control the electronic properties of the bilayer-graphene. In particular, the external fields significantly enhance the coupling of two Dirac cones, which result in additional or new van Hove singularities near the Fermi level. We compared the electronic structure of the orthorhombic stacking with those of AA and AB stackings. Our study may provide a deeper understanding of sliding effects of multilayer graphene. This work was supported by the Priority Research Center Program (2011-0018395) and the Basic Science Research Program through MEST/NRF (2013R1A1A2009131). This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

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