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Electronic properties of bilayer graphenes strongly coupled to interlayer stacking and an external electric field[1] CHANGWON PARK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JUNGA RYU, SUKLYUN HONG, Department of Physics and Graphene Research Institute, Sejong University, BOBBY SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GUNN KIM, Department of Physics and Graphene Research Institute, Sejong University, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — In the design of bilayer graphene (BLG)-based switching devices, it is critical to understand the complex stacking structures observed experimentally and their impact on the overall electronic properties. Using a maximally localized Wannier function, a highly accurate tight-binding Hamiltonian based on density functional theory was constructed and the stacking-dependent evolution of BLGs electronic band structures and their response to an external electric field were systematically investigated. Although the crossing band structures remain at any stacking configurations (i.e., no energy gap opens), the wavefunction characteristics around the Fermi level can differ qualitatively for different stackings. This difference is conveyed to energy gap opening properties in the presence of an external electric field. We, for the first time, established a phase diagram summarizing the stacking-dependent electronic structures of BLG, separating metallic and semiconducting characteristics for a given external field.

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