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Electronic structures transition for sliding bilayer graphene: A First-principles study[1] BI-RU WU, Department of natural science, Center for General Education, Chang Gung University — The weak interlayer interactions of bilayer graphene strongly affect the electronic structure in the low energy region. The stacking manner of graphene dominates the interlayer interaction and determines the band structure in the low energy region. However, the total energy difference between the most unstable AA stacked bilayer graphene and the most stable AB one is less than 5 meV per carbon atom. It means the sliding between the two layers of graphene is possible. We investigate the electronic structure transition of the sliding bilayer graphene via density functional theory. The graphene layer slides along the armchair and zigzag directions over whole unit cell are studied. The energy surface of the upper layer graphene sliding over whole unit cell reveals that the AA stacking manner has the highest energy and the AB stacked one has the lowest energy as expected, and one saddle point is observed for the AD stacked manner. For the electronic structure transition, the merging of Dirac points and gap opening are found during the sliding process.

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