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Electron-state engineering of bilayer graphene by sandwiching ionic molecules¹ NGUYEN THANH CUONG, MINORU OTANI, NRI-AIST, Tsukuba, Japan, SUSUMU OKADA, University of Tsukuba, Japan — Graphene has stimulated intense interest not only in the field of the low-dimensional sciences but also in the electronic device engineering because of its unique structural and electronic properties. In particular, they are regarded as a candidate material for the next-generation semiconductor devices. However, graphene is a metal with a pair of linear dispersion bands at the Fermi level, so that they are not utilized for the logic circuit. Therefore, it is important to tune the electronic structure and to get a semiconducting graphene. In this work, we demonstrate the possibility of controlling the band-gap and carrier type of bilayer graphene by using ionic molecules based on the first-principles total-energy calculations. Our calculations suggest that bilayer graphene sandwiched by a pair of cation and anion molecules is a semiconductor with a moderate energy gap of 0.26 eV that is attributable to the strong local dipole field induced by the ionic molecules. Furthermore, we also show that the carrier type of semiconducting bilayer graphene is controllable, i.e. intrinsic, p-type, or n-type semiconductors, by tuning anion-cation pair. [1].

[1] N. T. Cuong, M. Otani, and S. Okada, *Appl. Phys. Lett.* (2012), in press.

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