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Band engineering of bilayer graphene by metal atoms: First-principles calculations

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The continuous change in the electronic band structure of metal-adsorbed bilayer graphene was calculated as a function of metal coverage using first-principles calculations. Instead of modifying the unit cell size as a function of metal coverage, the distance between the metal atoms and bilayer graphene in the same 2×2 unit unit cell was controlled to change the total charges transferred from the metal atoms to bilayer graphene. The validity of the theoretical method was confirmed by reproducing the continuous change in the electronic band structure of K-adsorbed epitaxial bilayer graphene, as shown by Ohta et al. [Science 313, 951 (2006)] . In addition, the changes in the electronic band structures of undoped, n-type, and p-type bilayer graphene were studied schematically as a function of metal coverage using the theoretical method.