# Electronic property of bilayer graphene on pristine and rhenium-doped $MoS_2$

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Graphene, an exotic two-dimensional (2D) material, attracts great interest due to its precious properties. However, its gapless band structure becomes a limitation for electronic device applications. To date, several approaches are proposed to open a band gap in graphene.[1-3] In this work, first-principles calculation has been performed to investigate the electronic structure of bilayer graphene (BLG) on molybdenum disulfide ($MoS_2$) layer with and without rhenium (Re) atoms substitution and shows that a band gap is opened due to the build-in electric field.

Our results show that a band gap of 30 meV is opened for bilayer graphene on the surface of $MoS_2$ and the gap is enlarged to be 98 meV when one Mo atom is replaced by Re atom in the $MoS_2$. For the system without Re substitution, charge density analysis demonstrates that the existence of $MoS_2$ causes the charge redistribution of the bilayer graphene. The electron moves from the bottom layer of BLG and the top sulfur layer of $MoS_2$ to the intermediate region of these two layers, while there is no obvious charge density change around the top graphene layer. These charge distribution breaks the inversion symmetry of bilayer graphene, and induces a built-in electric field between two graphene layers, resulting in a small band gap.

For the system with Re substitution, Re dopant provides extra electron to $MoS_2$, inducing the charge transfer from $MoS_2$ to bilayer graphene. Charge density analysis shows that the charge depletion occurs near the bottom layer of graphene, however, the charge accumulation occurs near the top layer of graphene. Since the imbalance between charge distributions of bottom and top layers is increased, the built-in electric field is strengthened. Thus, the band gap of bilayer graphene is enlarged. In addition, our investigations also show that the band gap of monolayer graphene is not affected by the $MoS_2$ layer with and without Re substitution.

Our study reveals that the fundamental aspects of electronic properties in $MoS_2$ and BLG heterostructures toward their electronic device applications.

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[2] W.J.Zhang, et al., ACS NANO 5 (2011) 7517.

[3] B.N.Szafranek, et al., NANO Lett. 11 (2011) 2640.