Indirect bonding mechanism for proximity-induced giant spin-orbit coupling in graphene-topological insulator van der Waals heterostructure

SHIVANI RAJPUT, YAOYI LI, MICHAEL WEINERT, LIAN LI, Univ of Wisconsin, Milwaukee — We demonstrate proximity-induced spin-orbit coupling in graphene/topological insulator van der Waals (vdW) heterostructures fabricated by transferring chemical vapor deposited graphene onto Bi$_2$Se$_3$ film grown by molecular beam epitaxy. Using scanning tunneling microscopy/spectroscopy, we observe a spin-orbit splitting of the graphene Dirac states up to 80 meV, with a spatial variation of 20 meV due to the inherent lack of epitaxial relation in the graphene/Bi$_2$Se$_3$ vdW junction. Density functional theory calculations further reveal that this giant spin-orbit splitting of the graphene bands is a consequence of the orthogonalization requirement on the overlapping wave functions, rather than simple direct bonding at the interface. This revelation of an indirect bonding mechanism of the proximity effect will facilitate more effective engineering of desired properties in vdW heterostructures.

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