Exchange field and spin-orbit interaction induced band inversion in graphene on a TMD substrate

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Abstract We calculate the electronic band dispersion of graphene monolayer on a two dimensional transition metal dichalcogenide substrate (GTMD) (viz., XY_2 , X = Mo, W; Y = S, Se) around **K** and **K′** points taking into account the interplay of the exchange field due to the ferromagnetic impurities and the substrate induced, sub-lattice-resolved, strongly enhanced intrinsic SOCs. There are extrinsic Rashba spin-orbit coupling and the orbital gap related to the transfer of the electronic charge from graphene to XY_2 as well [1]. The former allows for external tuning of the band gap in GTMD and connects the nearest neighbors with spin-flip. On account of the strong spin-orbit coupling, the system acts as a quantum spin Hall insulator. The quantum anomalous Hall **s**tate could be accessed in this system through the introduction of the exchange field (M) by depositing Fe atoms on the graphene surface. Our graphical analysis with extremely low-lying states strongly suggests that GTMD exhibits band non-crossing at certain range of the exchange field value. In fact, in this case GTMD acquires a gap, making it behave as an insulator. At a critical value of the exchange field, the Dirac bands undergo spin-polarized band inversion (see Figure 1) due to the interplay of SOC and the exchange field. We have found this behavior is robust against an applied transverse electric field, and the vertical strain as long as the exchange field is tunable. Upon further increase of the exchange field, the gapped state becomes accessible once again. The cross-over alluded to above is quantum critical as it may occur at temperatures close to 0 K. A direct electric field control of magnetism at the nanoscale is needed here. The magnetic multiferroics, like $BiFeO_3$ (BFO), are useful for this purpose due to the coupling between the magnetic and electric order parameters.

References

[1] Z. Wang, D.-K. Ki, H. Chen, H. Berger, A. H. MacDonald,and A. F. Morpurgo, Nat. Commun. 6 (2015) 8339.

Figures

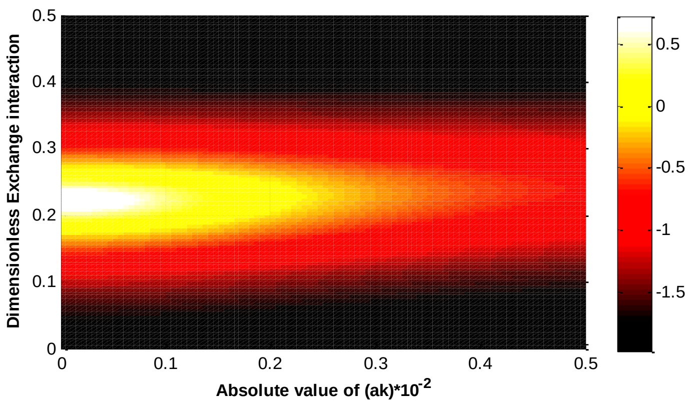

Figure1. The contour plot of Δn *(δ***k***, M)* as function of (*δk,M*). The function Δn is the difference in the occupation of the bands characterized by the indices ($\sigma = -1$, $s = +1$) and ($\sigma = +1$, $s = -1$). Here $\sigma = +1$ (–1) indicates the conduction (valence) band. Because of the spin-mixing driven by the Rashba coupling, the spin is no longer a good quantum number. Therefore the resulting angular momentum eigenstates are denoted by the spin chirality index $s = \pm 1$.The white-yellow (positive) region corresponds to the spin-polarized band-inversion. The red-hot and the dark regions correspond to the quantum spin Hall insulator.