Spin dynamics of graphene in heterostructure of graphene/TI system

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Abstract:

Recent studies pointed out that proximity to TI could enhance the spin-orbit coupling (SOC) strength in graphene and produce a topologically-protected state which is similar to that in TIs[1]. It is quite interesting to study such a heterostucture system of graphene and TI because it preserves both long spin lifetime[2] and the spin-momentum locking phenomenon on the graphene layer[3].

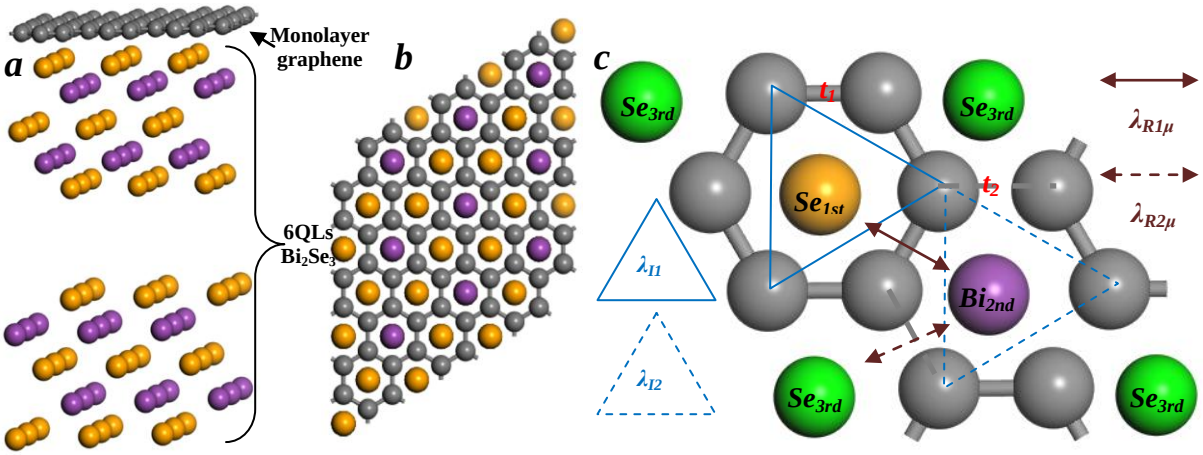

Figure 1 . Model of heterostructure of 6QL Bi_2Se_3/graphene. *a* – side view; *b* – top view; grey, khaki and purple colors indicate C, Se and Bi atoms respectively. *c* – TB parameters (t_1, t_2 – hopping; λ_{I1}, λ_{I2} – intrinsic SOC; $\lambda_{R1\mu}$, $\lambda_{R1\mu}$ – *rashba* SOC); khaki and green color indicate Se atom on 1st and 3rd layer respectively; while purple color indicates Bi atom on 2nd layer.

In this work, one monolayer of graphene with a √3 x √3 supercell was laid on top of a slab of TI with a thickness of six quintuple layers (QLs; shown in fig. 1a. & 1b.) in order to examine the electronic structure and the spin texture induced in graphene through DFT calculation (shown as red dash line in figure 2). According to figure 2a., the band gap of graphene is enlarged (~3.4 meV), due to the Kekulé C-C bonding distortion in the heterostructure and enhanced intrinsic SOC strength, and there is 2.8 meV *Rashba*-type splitting between bands as

well, which results from the out-of-plane *Rashba* SOC induced by TI film. On the other hand, expectation values of spin operator in figure 2*b*. ~ 2*d*. show that graphene holds an atypical *Rashba*-type spin texture with both non-zero out-of-plane and in-plane components and in-plane component shows a peak around every 45°; while out-of-plane component shows a peak around every 90°.

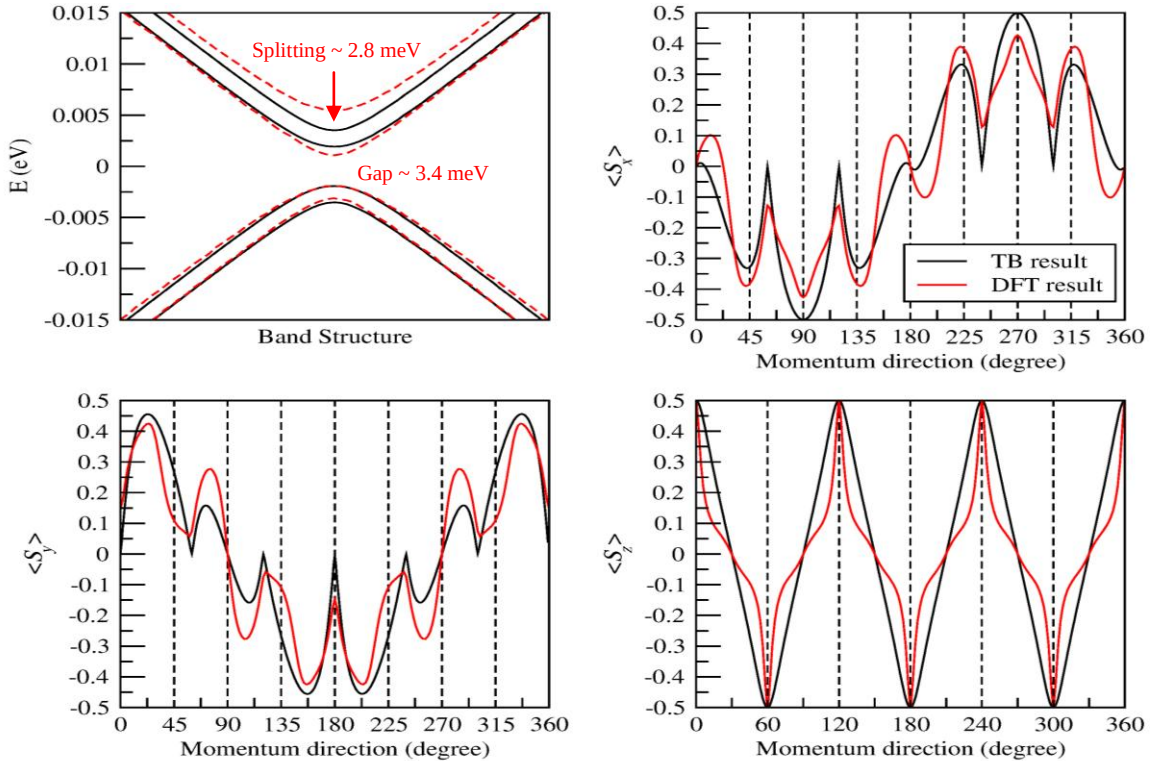

Figure 2. Electronic structure of graphene from DFT and TB calculations. *a* - band structure; *b* ~ *d* – expectation value of spin operator along three axes. t_1 = 2.646 eV; t_2 = (t_1 -2.529x10-3) eV; λ_{I1} = 0.532 meV; λ_{I2} = 0.444 meV; λ_{R1z} = 0.3 meV; λ_{R1i} = 3.333x10-3 meV; λ_{R2z} = -0.333 meV; λ_{R2i} = 1.0 meV

Then, a TB hamiltonain (illustrated in figure 1c. and results shown as black solid line in figure 2) was also generated, by fitting to the DFT band structure, and TB results show the same trend as DFT ones for the electronic structure. Based on this TB hamiltonian, the evolution of spin with time was computed to study the spin dynamics on the graphene layer. More details of the TB results and spin dynamics will be shown in following presentation and poster.

References:

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Year expected graduation: June, 2018
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