Proximity effects in graphene on alloyed transition metal dichalcogenides

Zahra Khatibi

Stephen Power School of Physics, Trinity College Dublin, Dublin 2, Ireland School of Physical Sciences, Dublin City University, Dublin 9, Ireland khatibiz@tcd.ie

Stacked heterostructures of graphene and transition metal dichalcogenides (TMDs) are particularly interesting for spin- and valleytronics since spin-orbit coupling (SOC) can be induced in the graphene layer by proximity effects with a strong valley dependence [1]. The induced proximity SOC, and associated imprinted spin-valley locking, enable experimentally verified spin-charge conversion and anisotropic spin relaxation effects that are absent in pristine graphene [2-3]. The nature and strength of the induced SOC depends on the composition of the TMD layer and its interaction with the graphene. Recent experimental advances allow the synthesis of TMD layers with a mix of metal atoms, suggesting that metal-atom alloving of the TMD layer may be an effective route to tune proximity effects in graphene-based heterostructures [4]. In this study we investigate the proximity induced SOC in graphene/TMD heterostructures by deliberate defecting of the TMD layer. We analytically study simple alloyed G/W_{1-x}Mo_xSe₂ heterostructures with diverse concentrations (x) and geometrical distribution of defects in the TMD layer. Utilizing density functional theory-computed electronic dispersions, spin textures, and an effective medium model, we evaluate the role of locally perturbed SOC on spin- and electronic signatures. We use the gained microscopic insight via tight-binding model to further examine the impact of defects in larger and more realistic heterostructures. We find that despite some dramatic perturbation of local SOC for individual defects, the low energy spin- and electronic behaviour yet follows the effective medium model. Since G/WSe₂ and G/MoSe₂ heterostructures individually maintain robust topological and trivial insulating phases, this finding yields that topological state of alloyed systems can be feasibly tuned via controlling the composition ratio of the metallic element.

References

M. Gmitra, Phys. Rev. B 93 (2016) 155104
A. W. Cummings, Phys. Rev. Lett. 119 (2017) 206601
L. A. Benítez, Nat. Phys 14 (2018) 303
F. A. Nugera, Small (2022), 2106600
Figures



Figure 1: (a) Schematic representation of a composite $G/W_{1-\chi}Mo_{\chi}Se_{2}$ heterostructure. The electronic dispersion of $G/W_{1-\chi}Mo_{\chi}Se_{2}$ with (b) $\chi=0$, (c) $\chi=0.67$, and (d) $\chi=1$.