Proximity effects in graphene on alloyed transition metal dichalcogenides

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Stacked heterostructures of graphene and transition metal dichalcogenides (TMDs) are particularly interesting for spintronics 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]. Recent high precision experiments based on currently available water-assisted CVD technique reveal composition-dependent band alignments in alloyed TMD lateral heterostructures with homogeneous intradomain composition [4]. Thus, in graphene/TMD heterostructures the nature and strength of the induced SOC depends on the composition of the underlying TMD layer. In this study we investigate the proximity induced SOC in graphene/TMD heterostructures by deliberate defecting of the TMD layer [5]. 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. Furthermore, we demonstrate that the topological state of such alloyed systems can be feasibly tuned by controlling this ratio.

References

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Figures

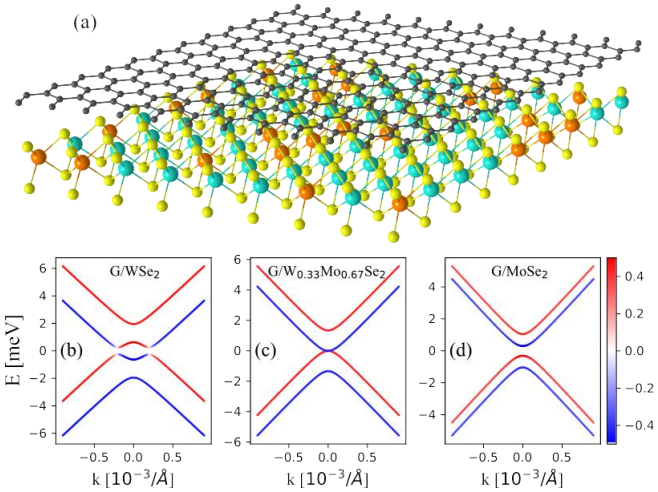

Figure 1: (a) Schematic representation of a composite graphene/TMDC heterostructure. [(b)–(d)] The proximity-induced band structure and topology transition for different TMDC layers.