The emergence of interface states in graphene/transition metal dichalcogenides heterostructure with lateral interface

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Proximity spin-orbit coupling in graphene on transition metal dichalcogenides (TMDC) is controlled via the metal composition in the TMDC layer [1]. While a graphene/$MoSe_2$, has a direct optical band gap driven by a sublattice asymmetric mass term, the proximity to WSe_2 leads to valley-Zeeman-driven inverted bands in a graphene/ WSe_2 heterostructure. Although topologically trivial with a vanishing Z_2 index, these systems can enable a topological crossover with band gap closure when placed together in a randomized composite graphene/TMDC system [2]. This is due to the non-zero Berry curvature at individual valleys and the change of the valley Chern index over a critical composition ratio. Therefore, inherently, a composite graphene/TMDC heterostructure can host localised boundary states given that W- and Mo-like domains with opposite valley Chern indices are formed. In this study we show that a graphene/(Mo-W)Se_2 heterostructure with lateral interface in the TMDC layer hosts topologically protected in-gap propagating modes similar to those at the border of commensurate AB and BA domains in a biased minimally twisted bilayer graphene [3-4]. Utilizing microscopic approaches, i.e. tight-binding model and ab initio calculations, we also demonstrate the evolution of the electronic dispersion with the system size from a weighted average effective model to zero energy branch crossings. Our findings show that, similar to previous studies [5], in the absence of intervalley scattering mechanisms, the topological interface states are robust.

References

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Figures

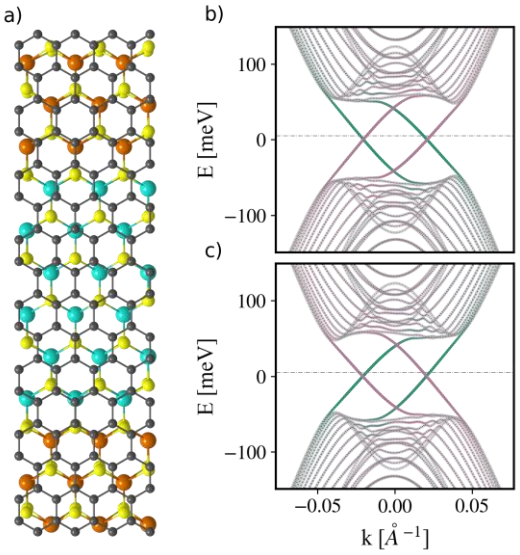

Figure 1: (a) DFT cell of a graphene/(Mo-W)Se_2 heterostructure with lateral interface in the TMDC layer. Tungsten, molybdenum, and carbon atoms are indicated by cyan, orange, and black spheres. The cell is equally divided into two graphene/$MoSe_2$ and graphene/WSe_2 regions and the domain walls are aligned with the zigzag direction. Different interfaces' contribution to the eigen value weight in a proximitized graphene with approximately 100 nm width around the (b) K and (c) K' valleys. The contribution of the first and second domain walls is depicted in green and purple colors, respectively.