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Topologically Protected Hybrid States in Graphene-Stanene-Graphene Heterojunction

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Section S1. Formation Energy and Adsorption Energy of C-Sn-C system.

To explore the chemical stability of heterostructure, we have calculated the formation energy for C-Sn-C system. We have considered the following equation[1];

$$\Delta E_{form} = E_{system} - N_{Sn} \times E_{Sn} - N_C \times E_C \quad \ldots 1$$

Where E_{system} is the total energy of the graphene-stanene-graphene system, E_{Sn} is total energy (per atom) of stanene, E_C is the total energy (per atom) of graphene, N_{Sn} is the total number of Sn atoms, and N_C is the total number of C atoms in the system. The calculated value of ΔE_{form} is -0.16 eV, which shows the stability towards the formation of graphene-stanene-graphene system. This may be due to the weak van der Waals interactions.

Section S2. Effect of length on the boundary states for armchair configuration.

In a ribbon, topological edge states are localized to the boundary of the ribbon. The hopping of charge from one edge to other edge is prohibited to prevent the interaction between edge states at the two different edges. At the same edge, two Kramers pairs are protected by time reversal symmetry[2]. Hence, they do not hybridize when cross each other. If the width of the ribbon is not sufficiently large, then the two edge states form will interact. Such an interaction can make the Dirac point massive by opening up a gap. Considering the armchair ribbon with three different ribbon lengths, we show that band gap decrease with increasing ribbon length. We have considered 8Å, 10.50Å and 12.95 Å armchair ribbon. The band gaps are 0.65eV, 0.16eV and 0.07eV respectively. So our results show that the band gap decreases with increasing ribbon width.

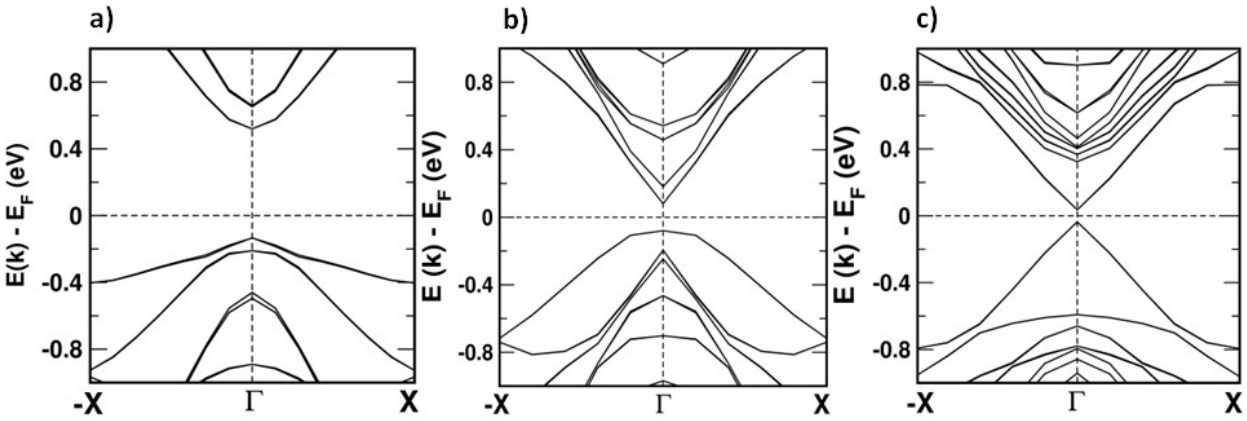

Figure S1: Boundary states for different arm-chair ribbons; a) 8.00Å, b) 10.50Å and c) 12.95Å

References:

1. Hong, J. et al. Exploring atomic defects in molybdenum disulphide monolayers. Nat. Commun. **2015**, 6, 6293.
2. Kane, C. L. and Mele, J. E. Quantum Spin Hall Effect in Graphene. Phys. Rev. Lett. **2005**, 95, 226801.