

Abstract Submitted  
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**Van der Waals Stacking Induced Topological Phase Transition in Layered Ternary Transition Metal Chalcogenides<sup>1</sup>** XIAOFENG QIAN, Department of Materials Science and Engineering, Texas A&M Univ. — Novel topological materials are key to the development of topological devices with low power consumption and heat dissipation. Here we theoretically predict that a novel class of ternary transition metal chalcogenides exhibit dual topological characteristics: quantum spin Hall insulators (QSHIs) in 2D monolayers and topological Weyl semimetals in vdW stacked noncentrosymmetric bulk. Remarkably, one can create and annihilate Weyl fermions, and realize the transition between Type-I and Type-II Weyl fermions by tuning vdW interlayer spacing, based on which we provide the missing physical picture of the evolution from 2D QSHIs to 3D Weyl semimetals. Our results show that these materials are thermodynamically stable with weak interlayer binding, implying their great potentials for experimental synthesis, characterization, and vdW heterostacking. Their ternary nature will offer more tunability for electronic structure by controlling different stoichiometry and valence charges. These new materials provide an ideal platform for exploring fundamental topological phase transition, and will open up a variety of new opportunities for 2D and topological materials research. (Reference: Junwei Liu, Hua Wang, Chen Fang, Liang Fu, and Xiaofeng Qian. arXiv preprint arXiv:1606.04522 (2016))

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