

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Rhombohedral Sb_2Se_3 as an intrinsic topological insulator due to strong van der Waals inter-layer coupling GUOHUA CAO, HUIJUN LIU, Wuhan University, ZHENYU ZHANG, University of Science and Technology of China — Topological insulators are a new class of quantum materials, which have insulating energy gaps in bulk form, but exhibit robust gapless surface states. It was theoretically predicted and experimentally confirmed that the binary tetradymites Bi_2Te_3 , Bi_2Se_3 , and Sb_2Te_3 are three-dimensional topological insulators. In this talk, we demonstrate by first-principles approach that the prevailingly believed trivial system of Sb_2Se_3 with relatively weaker spin-orbital coupling, is actually also a topological insulator, as characterized by its topologically protected surface states and the Z_2 invariant. The underlying reason is the ubiquitous van der Waals interaction between quintuple layers. We also generalize our considerations to several related systems in an attempt to draw generic guiding principles.

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Date submitted: 10 Nov 2016

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