

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Emergence of topological semimetals in gap closing in semiconductors without inversion symmetry SHUICHI MURAKAMI, MOTOAKI HIRAYAMA, RYO OKUGAWA, Tokyo Inst of Tech - Tokyo, TAKASHI MIYAKE, AIST, Tsukuba, Japan — In this presentation, we show emergence of topological semimetals in gap closing of any inversion-asymmetric insulators. Namely, we begin with any inversion-asymmetric insulators, and close a gap by changing a parameter in the system; we then show that the system becomes either (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, both are among topological semimetals. In particular, no insulator-to-insulator transition happens, in strong contrast with inversion-symmetric systems. This result also has implications for Z_2 topological number. In a transition between different Z_2 topological phases, a Weyl semimetal phase necessarily appears when inversion symmetry is broken, for materials with any space groups [1,2]. Our theory is applicable to many materials, for example to tellurium (Te) [3]. Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. [1] S. Murakami, *New J. Phys.* 9, 356 (2007). [2] S. Murakami, M. Hirayama, R. Okugawa, T. Miyake, arXiv:1610.07132. [3] M. Hirayama, R. Okugawa, S. Ishibashi, S. Murakami, T. Miyake, *Phys. Rev. Lett.* 114, 206401 (2015).

Shuichi Murakami
Tokyo Inst of Tech - Tokyo

Date submitted: 11 Nov 2016

Electronic form version 1.4