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Symmetry-based Search for Topological Weyl Nodes and Nodal-lines in Realistic Materials MOTOAKI HIRAYAMA, SHUICHI MURAKAMI, Dept. of Physics, Tokyo Tech.; TIES, Tokyo Tech., RYO OKUGAWA, Dept. of Physics, Tokyo Tech., SHOJI ISHIBASHI, TAKASHI MIYAKE, CD-FMat, National Institute of Advanced Industrial Science and Technology — Topological semimetals such as Weyl semimetals and nodal-line semimetals have been under intensive investigation recently. In this study, to realize such semimetals, we start from any insulators without inversion symmetry, and assume that the gap closes by changing some parameter. We then show that after the gap-closing there are only two possibilities; one is a Weyl semimetal phase, and the other is a nodal-line semimetal, depending on the symmetry and the position of the gap-closing point. Our analysis tells us which cases lead to Weyl semimetal and to the nodal-line semimetal, and this result can be used to find realistic topological semimetals. As an example, we study tellurium [1] using ab initio calculation based on relativistic density functional theory. The electronic structure is calculated by OpenMX [2] and the structural optimization is executed by QMAS [3]. We find that HfS has the nodal line in the mirror symmetry plane, and the nodal-line vanishes by pressure or atomic substitution. We also propose some materials showing the spinless nodal lines and its topological surface states. [1] M. Hirayama, R. Okugawa, S. Ishibashi, S. Murakami, and T. Miyake, Phys. Rev. Lett. 114, 206401 (2015). [2] http://www.openmx-square.org/ [3] http://www.qmas.jp/

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