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Weyl Nodes in Trigonal Tellurium and Selenium MOTOAKI HIRAYAMA, Nanosystem Research Institute, AIST, RYO OKUGAWA, Department of Physics, Tokyo Institute of Technology, SHOJI ISHIBASHI, Nanosystem Research Institute, AIST, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology; TIES, Tokyo Institute of Technology, TAKASHI MIYAKE, Nanosystem Research Institute, AIST — Singular points in the momentum space (Dirac nodes) have been under intensive investigation recently. Among various Dirac systems, materials having three-dimensional Dirac nodes without spin degeneracy (Weyl nodes) are of particular interest because of their topological nature. We study trigonal Te and Se as systems having both strong spin-orbit interaction (SOI) and broken inversion symmetry, which is necessary for the Weyl node. We calculate the electronic structure by using QMAS [1] based on relativistic density functional theory, and add the self-energy correction in the GW approximation. Te and Se are insulating at ambient pressure. The conduction bands have a spin splitting similar to the Rashba splitting around the H points, but unlike the Rashba splitting the spin directions are radial, forming a hedgehog spin texture. The energy gap decreases with increasing pressure. In the metallic phase, the spin rotates twice around H on the $k_z = \pm\pi/c$ plane, which can be explained by the motion of the Weyl nodes under pressure [2]. We also find that trigonal Te shows the Weyl semimetal phase with time-reversal symmetry under pressure [2].

[1] http://www.qmas.jp/
[2] M. Hirayama, R. Okugawa, S. Ishibashi, S. Murakami, and T. Miyake: arXiv 1409.6399.

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