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**Spin-Orbit Effect on Dirac Cone in Selenium and Tellurium under Pressure** MOTOAKI HIRAYAMA, SHOJI ISHIBASHI, TAKASHI MIYAKE, NRI, AIST — We study the electronic structures of the group-VI elements, Se and Te, from first-principles in the local spin density approximation with the GW self-energy correction included. Both Se and Te are gapful at the ambient pressure. We use the Quantum MAterials Simulator (QMAS) package for the calculation with the spin-orbit interaction [1], and the full-potential linear muffin-tin orbitals method for the calculation of the non-relativistic self-energy. The calculated band gap is in excellent agreement with experiments, where the spin-orbit interaction substantially reduces the gap. The materials undergo an insulator-to-metal transition under pressure. In the metallic phase, at a certain pressure, two conducting states appear at around the H point, and they cross each other near the Fermi level. If the spin-orbit interaction is neglected, the states have linear dispersion in the vicinity of the crossing point, forming Dirac cone. The band crossing is protected even in the presence of spin-orbit interaction by the helical structure with the threefold symmetry. The spin structure at the H-point is peculiar: The spins for all non-degenerate states are confined in the ab plane, and points to the radial direction. [1] http://www.qmas.jp/

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