Multiple Dirac points and surface nonlinear optics in topological semimetal $HfGe_{0.92}Te$

Long CHEN[1,2], Qiming ZHAO[3], Liqin ZHOU[1,2], Ying ZHOU[1,2], Fei LIANG[3], Chen LIU[4], Jia'ou WANG[4], Shuxian WANG[3], Hongming WENG[1,2], Haohai YU[3], Gang WANG[1,2]*.

*lead presenter: gangwang@iphy.ac.cn

1 Institute of Physics, Chinese Academy of Sciences, China
2 University of Chinese Academy of Sciences, China
3 Shandong University, China
4 Institute of High Energy Physics, Chinese Academy of Sciences, China

The topological material with Dirac points having linear dispersions near the Fermi level has been a fascinating topic in condensed matter physics and materials physics. Here we report the band structure and surface nonlinear optics of topological semimetal $HfGe_{0.92}Te$ single crystal, which crystallizes in a tetragonal space group *P*4/*nmm* (No. 129) with about 8% vacancy on the Ge square net. By using angle-resolved photoemission spectroscopy (ARPES), the Dirac nodal line composed of the conventional Dirac points vulnerable to spin-orbit coupling (SOC) is observed, accompanied by the robust Dirac points protected by the nonsymmorphic symmetry against SOC and Ge vacancies. In particular, spin-orbit Dirac points originating from the surface state under the significant SOC could exist according to ARPES and first-principles calculations. Furthermore, $HfGe_{0.92}Te$ exhibits a remarkable surface second-order nonlinear susceptibility up to $5535 \pm 308\ \mathrm{pm \cdot V^{-1}}$. The surface nonlinear conversion efficiency is optimized to 3.75‰ using the angular engineering strategy, which is comparable to the well-designed optical waveguides and higher than the typical low-dimensional materials and metamaterials. The applicable frequency doubling wavelengths are extended from the visible region to the deep ultraviolet region ($\lambda_{2\omega}$ from 779 nm to 257.5 nm) with comparable conversion efficiency due to its linear dispersion in a wide energy range near the Fermi level and small chemical potential.