Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Stable Dirac semi-metal in the allotrope of IV elements PEIZHE TANG, Stanford Univ, WENDONG CAO, Tsinghua Univ, SHOU-CHENG ZHANG, Stanford Univ, WENHUI DUAN, Tsinghua Univ, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science,, ZHANG'S GROUP COLLABORATION, ANGEL'S GROUP COLLABORATION, DUAN'S GROUP COLLABORATION — Three dimensional (3D) topological Dirac semi-metals (SM) represent a novel state of quantum matter with exotic electronic structures, in which a pair of Dirac points with the linear dispersion along all three momentum directions exist in the bulk and are protected by the rotation symmetry. Regarded as the copies of 3D Weyl SMs, the Dirac SMs possess unique Fermi-arcs with helical spin textures on some specific surface planes. Herein, by using first principles calculations with the hybrid functional, we discover a new metastable allotrope of Ge and Sn with the staggered layered dumbbell structure, named as germancite and stancite, to be 3D Dirac SMs with a pair of Dirac points on the rotation axis of C_3. On the surface parallel to the rotation axis, a pair of topologically non-trivial Fermi arcs are observed to be coexisting with the trivial surface states; and via tuning the Fermi level, the hybridization between them induces a Lifshitz transition on the Fermi surface. Furthermore, the quantum thin film of the germancite is found to be the quantum spin Hall insulator without applying external electric field. These discoveries explore the metastable allotrope of Ge and Sn as topological Dirac SMs showing novel physical properties and future applications.

Peizhe Tang
Stanford Univ

Date submitted: 05 Nov 2015 Electronic form version 1.4