Massachusetts Institute of Technology
Department of Physics

INFORMAL CONDENSED MATTER SEMINAR

"2D and 3D Topological Crystalline Insulators in IV-VI Semiconductors"

Junwei Liu
Tsinghua University and MIT

Abstract: Topological crystalline insulators (TCI) are new topological phases of matter protected by crystal symmetry of solids. Based on ab-initio calculation and KP theory, we predicted that SnTe and the related alloy $Pb_{1-x}Sn_x$(Te, Se) can be 3D TCI, which are quickly confirmed in experiments. Based on the microscopic understanding of bulk-boundary correspondence in TCI, we explicitly derive the KP Hamiltonian for TCI surface states from the electronic structure of the bulk and find **two types** of surface states with qualitatively different properties depending on the surface orientation. In particular, we predict that (111) surface states consist of four Dirac cones centered at time-reversal-invariant momenta {Γ} and M; while (001) and (110) surface states consist of Dirac cones at non-time-reversal-invariant momenta. Moreover, both (001) and (110) surface states exhibit a Lifshitz transition as a function of Fermi energy, which is accompanied by a Van-Hove singularity in density of states arising from saddle points in the band structure. The different properties of the two types of surface states result in very different topological phenomena for the related thin film grown along different direction. Typically, (001) thin film can be 2D TCI and (111) thin film can be 2D TI. Both exist in an extensive thickness range and possess huge non-trival band gap above 50 meV.

3:30 PM
Wednesday, April 10, 2013
Room 4–331