Condensed Matter Theory Seminar

"Nonlinear electrical and optical response in Weyl semimetals"

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Abstract: Noncentrosymmetric metals are anticipated to exhibit a second order Hall likecurrent in the nonlinear electrical response caused by the Berry curvature dipole in momentum space. Weyl semimetals (WSMs) are expected to be excellent candidates for observing these nonlinear effects because of Berry curvature monopole. We have implemented the semiclassical Berry curvature dipole formalism into an ab initio scheme and investigated the second-order nonlinear response for three representative groups of materials: the TaAs-family type-I WSMs, MoTe2-family type-II WSMs and their monolayer structures. Both types of WSMs exhibited a strong Berry curvature dipole, in which type-II Weyl points are usually superior to the type-I because of the strong tilt.

I would also introduce the second order Kubo approach for investigating the nonlinear optical response in TaAs with ab-initio Hamiltonian. Our calculations reveal that the photocurrent is predominantly contributed by the three-band transition from the occupied Weyl band to the empty Weyl band via an intermediate band away from the Weyl cone, for excitations both by linearly and circularly polarised lights. Our work provides the first first-principles calculation on nonlinear optical phenomena of Weyl semimetals and serves as a deep understanding of the photogalvanic effects in complexed materials.

12:00pm noon Wednesday, November 7, 2018 Duboc Room (4-331)