Density wave driven metal-insulator transition in nickelates
SUNGBIN LEE, RU CHEN, University of California, Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, BALENTS GROUP TEAM — The Mott transition in nickelates, RNiO3, shows unusual magnetic ordering and charge ordering in the insulating phase. For the more itinerant nickelates, one may argue that these unusual density waves are actually driven by Fermi-surface nesting, originated from the large flat regions of Fermi surfaces. Using a tight-binding model of the band derived from doubly degenerate eg orbitals, we obtain the density wave induced metal-insulator transition phase diagram in the presence of on-site Coulomb interaction and Hund’s coupling, treated in Hartree-Fock approximation. Furthermore, motivated by recent success in layer by layer growth of nickelates, the thin film effects in nickelates are also studied. Finally we calculate the optical conductivity for the various states in our phase diagram, suggesting experimental measurements to check the theory.