Mott transition in three-dimensional nodal semimetals

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The molecular antiferromagnet, (ET)Ag4(CN)5 and the molecular conductor [Pd(dddt)2] are benchmark systems for studying the behavior of electrons in nodal semimetals. The interplay between kinetic energy, spin-orbit coupling and Coulomb repulsion can lead to topological phases such as the topological Mott or the Weyl-Mott insulator which are under intense exploration.

In the present Master project, we will study the Mott transition in a half-filled diamond lattice which is a nodal semimetal when no Coulomb interaction is present. By using the dynamical mean-field theory framework we will study the effect of Coulomb repulsion on these lattices focusing on their topological properties across the Mott transition. The results will shed light on the Mott insulator to Dirac semimetal transition observed in (ET)Ag4(CN)5 under pressure and the unconventional electronic transport observed in [Pd(dddt)2].