MAR14-2013-000438

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Topological phases in mix valence compounds

XI DAI, Institute of Physics, Chinese Academy of Sciences

In this talk, I will propose that the mix valence phenomena in some of the rare earth compounds will naturally lead to non-trivial topology in band structure.One of the typical example is SmB6, where the intermediate valence of Sm generates band inversion at the X point and the non-trivial Z2 index. Other than SmB6, YbB6 and YbB12 are both mix valence compounds. By applying LDA+Gutzwiller to these materials, we find that YbB6 has non-trivial Z2 index, indicating that YbB6 is another three dimensional topological insulator with strong correlation effects. Our calculation also finds that YbB12 is a trivial insulator in the sense of Z2 but it can be classified as topological crystalline insulator with non-zero mirror Chern number. The electronic structure at finite temperature has also been studied using LDA+DMFT, indicating YbB6 is still in the mix valence region while YbB12 is quite close to the Kondo limit.