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■ 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.

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2006 6 (Rutgers) 2004 6 1999 2004
2009.10 LDA Gutzwiller
NaCoO₂ Ce Bi₂Se₃
2010 2013 3
Cr Bi₂Te₃
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