

Massachusetts Institute of Technology  
Department of Physics

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**Condensed Matter Theory Seminar**

**“Topological Phases in Mix Valence Compounds”**

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**Abstract:** 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 SmB<sub>6</sub>, where the intermediate valence of Sm generates band inversion at the X point and the non-trivial Z<sub>2</sub> index. Other than SmB<sub>6</sub>, YbB<sub>6</sub> and YbB<sub>12</sub> are both mix valence compounds. By applying LDA+Gutzwiller to these materials, we find that YbB<sub>6</sub> has non-trivial Z<sub>2</sub> index, indicating that YbB<sub>6</sub> is another three dimensional topological insulator with strong correlation effects. Our calculation also finds that YbB<sub>12</sub> is a trivial insulator in the sense of Z<sub>2</sub> 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 YbB<sub>6</sub> is still in the mix valence region while YbB<sub>12</sub> is quite close to the Kondo limit.

**2:30 pm**  
**Monday, November 25, 2013**  
**Duboc Seminar Room (4-331)**