Tata Institute of Fundamental Research
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Seminar

Mott insulators induced by hybridization switching in ABO_3 perovskites

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Model Hamiltonians for strongly correlated oxides of the type ABO_3, typically ascribe a secondary role to the A sites. They are assumed to be simple agencies for controlling bandwidth, doping, disorder etc., while the real action is expected to take place, either at the transition metal (B) sublattice or at the B-oxygen sublattice. However, we will show that the stability of the Mott phase, in oxides with valence skipping A site elements (e.g. $PbCoO_3$, $BiNiO_3$), depends on both B-site strong correlation and A-oxygen hybridization. For this, we will introduce a Hamiltonian involving all three species and study its zero temperature properties within a slave rotor mean field approach. We will describe how a hybridization switching instability between the A site and oxygen conspires with strong correlation on the B site to stabilize a Mott insulator at ambient pressure. Further, by modeling pressure effects in the slave rotor theory (with inputs from ab initio electronic structure calculations), we will explain the observed pressure induced insulator to metal transition in these oxides*.

Tuesday, Feb 19th 2019

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H