Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electronic Structure and Magnetism of Ir based Oxides[1] INDRA DASGUPTA[2], Department of Solid State Physics, SWARUP PANDA[3], None — We have investigated in details the electronic structure of several Ir based oxides where in addition to crystal field and Coulomb repulsion, the spin-orbit coupling (SOC) plays an important role. We shall first consider two Ir based oxides with 4+ (d^5) charge state of Ir, namely the insulating double perovskite Sr_2CeIrO_6 and the metallic rutile IrO_2, and examine the validity of the novel spin-orbital entangled J_{eff}=1/2 states for the description of their electronic structure. In particular, explore in details whether the J_{eff}=1/2 state survives for the itinerant metallic IrO_2. Finally we shall also present our electronic structure calculations on 6H perovskite type iridates where different charge state of Ir (5+, 4.5+, and 4+) may be realized. We show in addition to SOC, the strong intra-dimer hopping play a crucial role for the magnetic ground state and the insulating property of these systems. We shall compare our results with available experiments.

[1]The authors thank Department of Science and Technology, Govt. of India, for financial support.
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Date submitted: 14 Nov 2013 Electronic form version 1.4