

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**A New Class of  $J_{eff} = 1/2$  Mott Insulators** TURAN BIROL, KRISTJAN HAULE, Rutgers, The State University of New Jersey — We predict a novel class of  $J_{eff}=1/2$  Mott insulators in a family of Ir and Rh fluoride compounds with the  $K_2GeF_6$  crystal structure that are previously synthesized, but not characterized extensively. First principles calculations in the level of all electron Density Functional Theory + Dynamical Mean Field Theory (DFT+DMFT) indicate that these compounds have large Mott gaps and some of them exhibit unprecedented proximity to the ideal,  $SU(2)$  symmetric  $J_{eff}=1/2$  limit.

Turan Birol  
Rutgers, The State University of New Jersey

Date submitted: 11 Nov 2014

Electronic form version 1.4