Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Effective J=1/2 insulating state in Ruddlesden-Popper iridates: An LDA+DMFT study HONGBIN ZHANG, KRISTJAN HAULE, DAVID VANDERBILT, Rutgers Univ — Using *ab-initio* methods, we[1] investigate the metal-insulator transition across the Ruddlesden-Popper (RP) iridates and explore the robustness of the effective $J = 1/2$ insulating state[2] against band effects due to itineracy, tetragonal distortion, octahedral rotation and Coulomb interaction. The electronic structures we obtained are in good agreement with recent ARPES measurements.[3,4,5] We predict the effects of epitaxial strain on the optical conductivity, magnetic moments and effective $J = 1/2$ ground-state wave functions in the RP series. We demonstrate that the deviation from the ideal effective $J = 1/2$ state is negligible at short time scales for both Sr_2IrO_4 and $Sr_3Ir_2O_7$, while it becomes quite significant for $Sr_3Ir_2O_7$ at long times and low energy, leading to a reconciliation of previous contradictory experimental results.

[1]H. Zhang, K. Haule and D. Vanderbilt, arXiv:1308.4471 (2013).
[2]B.J. Kim *et al.*, Phys. Rev. Lett. **101**, 076402 (2008).
[3]B.M. Wojek, *et al.*, J. Phys.: Condens. Matter **24**, 415602 (2012).
[4]Q. Wang, *et al.*, Phys. Rev. B **87**, 245109 (2013).
[5]Y. Nie, P. King, and K. Shen, private communication.

Hongbin Zhang
Rutgers Univ

Date submitted: 13 Nov 2013 Electronic form version 1.4