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, we¹ investigate the metal-insulator transition across the Ruddlesden-Popper (RP) iridates and explore the robustness of the effective J = 1/2 insulating state² 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 Sr₂IrO₄ and Sr₃Ir₂O₇, while it becomes quite significant for Sr₃Ir₂O₇ at long times and low energy, leading to a reconciliation of previous contradictory experimental results.

 $^1\mathrm{H.}$ Zhang, K. Haule and D. Vanderbilt, arXiv:1308.4471 (2013).

²B.J. Kim *et al.*, Phys. Rev. Lett. **101**, 076402 (2008).

³B.M. Wojek, et al., J. Phys.: Condens. Matter 24, 415602 (2012).

⁴Q. Wang, et al., Phys. Rev. B 87, 245109 (2013).

⁵Y. Nie, P. King, and K. Shen, private communication.

Hongbin Zhang Rutgers Univ

Date submitted: 13 Nov 2013

Electronic form version 1.4