Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic, magnetic and optical properties of $\mathbf{Sr_{n+1}Ir_nO_{3n+1}}$ (n=1, 2, and ∞)[1] PEITAO LIU, Faculty of Physics, University of Vienna, Vienna, Austria, SERGII KHMELEVSKYI, Department of Applied Physics, Vienna University of Technology, Vienna, Austria, BONGJAE KIM, Faculty of Physics, University of Vienna, Vienna, Austria, XING-QIU CHEN, DIANZHONG LI, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China, CESARE FRANCHINI, Faculty of Physics, University of Vienna, Vienna, Austria — We have studied the crossover between metallic/insulating and non-magnetic/magnetic phases in Ruddlesden-Popper series of iridates $Sr_{n+1}Ir_nO_{3n+1}$ (n=1, 2, and ∞) by means of density functional theory including an on-site Hubbard U correction and many-body first principles methods. By systematically investigating the evolution of the orbital and spin properties as a function of U, spin-orbit coupling (SOC) strength, and n we have constructed detailed phase diagrams of the metal-insulator transition (MIT) which provide clear evidence for the crucial role played by SOC and U in establishing a relativistic Mott-Hubbard insulating state in the n=1 and 2 compounds. Optical spectra computed within a model Bethe-Salpeter scheme show the typical double peak structure observed in experiments and capture well the progressive shrinking of the band-gap and the widening of the bandwidth going from n=1 to n=∞. Finally, we clarify the origin of the canted magnetic ground state of Sr_2IrO_4 as due to the the synergistic effect of structural distortions (rotation and tetragonal distortion of IrO_6 octahedral) and to the competition between exchange and Dzyaloshinskii-Moriya interactions.

[1]This work is supported by the China Scholarship Council and Austria Science fund.

Peitao Liu
Faculty of Physics, University of Vienna, Vienna, Austria

Date submitted: 14 Nov 2014 Electronic form version 1.4