Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic structure of La_2CuO_4 within self-consistent GW approximation SANGKOOK CHOI, Rutgers University, Piscataway, NJ, USA, ANDREY KUTEPOV, Ames Laboratory, Ames, IA, USA, KRISTJAN HAULE, Rutgers University, Piscataway, NJ, USA, MARK VAN SCHILFGAARDE , King's college, London, UK, GABRIEL KOTLIAR, Rutgers University, Piscataway, NJ, USA — La_2CuO_4, the parent compound of the high-temperature superconductor, is a classic strongly-correlated material. We present a first-principles study on the excitations spectrum of La_2CuO_4 within the self-consistent GW approximation based on full-potential linearized augmented-plane-wave methods. We compare the results of the Quasiparticle (QP) self-consistency and the fully self consistent approach. We find that the spin-polarized self-consistent GW calculation succeed in predicting the insulating ground state and anti-ferromagnetic ordering. It also describes charge-transfer character of the top of the valence band and reproduce the experimental spectral function well, including the weight of the copper d and the position of the lanthanum levels, but it overestimates the bandgap by 75%. We comment on the implications of our results for the implementation of GW+DMFT in a one shot, QP, and fully self consistent version.

Sangkook Choi
Rutgers University, Piscataway, NJ

Date submitted: 14 Nov 2014 Electronic form version 1.4