Planar-coordinated nickelates, isoelectronic to overdoped cuprates: an LDA+DMFT comparison

CHUCK-HOU YEE, GABRIEL KOTLIAR, KRISTJAN HAULE, Rutgers University — We show the Ni-O planes in the bilayer and trilayer T'-type nickelates, recently synthesized by Poltavets, et al. [1], are electronically analogous to the Cu-O planes in overdoped superconducting cuprates. The density of states, Fermi surface, nickel valence and mass renormalization, computed using LDA+DMFT, are in good agreement with available experiment, and indicate that the compounds are well-described by multilayer Hubbard physics. Significant interlayer coupling generates bonding-antibonding Fermi surfaces, similar to those seen in the cuprates. We investigate the possibility that interlayer coupling can explain the presence of a phase transition with $R \log 2$ entropy in the trilayer, and the absence of such a transition in the bilayer.