Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electronic properties and chain conductivity of underdoped $YBa_2Cu_3O_{6+x}$ by First-Principles calculations VINCENZO FIORENTINI, ALESSIO FILIPPETTI, GIORGIA LOPEZ, MAURO MANTEGA, University of Cagliari, Italy — Metal-insulating transitions in cuprates represent an historical challenge for first-principles calculations. Here we present results obtained through the pseudo-self-interaction free density functional scheme (PSIC) that is capable to correct the gross failures of LSDA at just a moderate increase of computing effort, and works well in both strong-correlated and metallic limit. Here we describe the properties of the end-point systems $YBa_2Cu_3O_6$ and $YBa_2Cu_3O_7$ as well as the chemistry of insulating-metal transition occurring in the CuO chains of underdoped $YBa_2Cu_3O_{6+x}$ in the region x=[0,0.5]. Coherently with the one-dimensional metallic percolative regime observed at low-doping, we find that the metal-insulating transition occurring at low doping in the non-magnetic Cu(1)Ox chains is induced by chain-like alignment of the doping oxygens within the chains, whereas disorder (i.e. non chain-aligned) distributions are always insulating. In the Cu(2)O2 planes the insulating antiferromagnetic state remains stable up to x=0.25, while at x=0.5 a normal-metal state, similar to that seen for $YBa_2Cu_3O_7$, take place. The in-plane antiferromagnetic- paramagnetic competition depends on x but is almost unaffected by the intra-chain order-disorder competition.

Alessio Filippetti
University of Cagliari, Italy

Date submitted: 29 Nov 2007 Electronic form version 1.4