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Metal-insulating phase transition in $YBa_2Cu_3O_{6+x}$ by First-Principles ALESSIO FILIPPETTI — The basic chemistry of $YBa_2Cu_3O_{6+x}$ represents an hystorical challenge for first-principles approaches, due to the well known difficulty of standard local-spin density functional theories (such as LSDA or GGA) in describing the correct spin-polarized S=1/2 ground-state of Cu (II) ion. Here we employ the pseudo-SIC approach, which is based on an approximate form of self-interaction corrected (SIC) Kohn-Sham Equations and works well in both Mott-insultaing (i.e. x=0) and metallic limit (x=1), to describe the effect of oxygen-doping on the electronic properties of $YBa_2Cu_3O_{6+x}$. Our results give a sound description of the order-disorder as well as magnetic-non magnetic phase competitions. We show that the phase transition from the antiferromagnetic insulating to the paramagnetic metal is mainly governed by the ordering of doping oxygens in Cu(I)-O-Cu(I) chains, which in turn, subtly affects the chemistry of Cu(II)-O_2 planes through a non trivial pattern of p-d couplings.

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