Electronic reconstruction and surface two dimensional electron gas in the polarized heterostructure with hole doped single copper-oxygen plane

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We propose a novel structure with a symmetrical CuO_2-relative structural subunit [SrO-La_2CuO_4-SrO] sandwiched between polar $LaAlO_3$ (LAO) and nonpolar $SrTiO_3$ (STO), which has the needed internal field for hole doping in the CuO_2 plane. This structure is studied to get some insight into the evolution from antiferromagnetic (AFM) state to superconducting state and to identify the possible role of disorder. The polarization in the LAO part is the ideally cleanest source with strength as high as ~ 10^9 V/m, and is the origin of a controllable hole doping and metallic surface state in the designed disorder-free heterostructure (HS). The hole concentration can be rationally manipulated by tuning the $LaAlO_3$ thickness and in-plane strain. Although we find magnetic states have an unstable trend, the AFM state is still magnetic ground state up to the 8% doping level, which reveals the possible role of chemical disorder in destroying charge order, orbital order, and finally magnetic order of bulk hole doped La_2CuO_4. Moreover, this AFM insulating state co-exists with a surface two dimensional electron gas, which originates from out-of-plane charge (holes) transport mainly between the La-d_{3z2-1} state at the surface and Cu-e_g states in the CuO_2 plane. In addition, a possible $SrTiO_3$ capping layer is introduced, in which, instead of La-d_{3z2-1}, Ti-t_{2g} orbitals exchange holes with electrons of Cu-e_g orbitals.

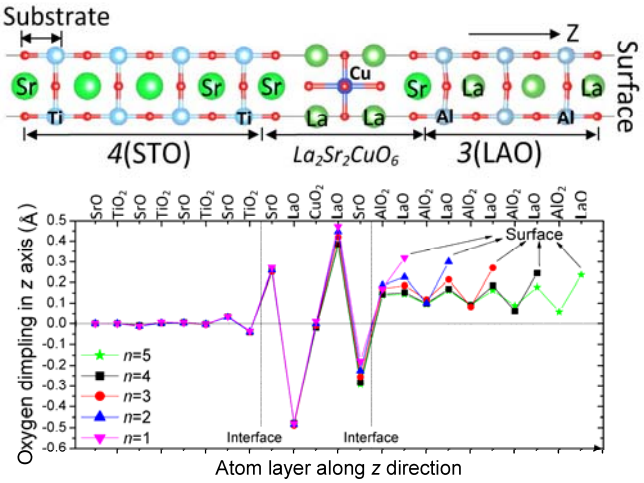

Fig. 1 Top panel: Schematic geometrical structures of 4(STO)/$La_2Sr_2CuO_6$/3(LAO) HS. Bottom panel: Calculated oxygen dimpling away from cation planes for 4(STO)/$La_2Sr_2CuO_6$/*n*(LAO) HSs (1≤n≤5) in *z* direction.

References:

[1] Xiaoping Yang, Haibin Su, accepted by Phys. Rev. B