Orbital character of the mobile and localized electron states at the LAO/STO interface

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The discovery of high mobility two-dimensional electron system (2DES) emergent at the interface between two wide band-gap insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) has put forward new perspectives of oxide electronics where interfacing different materials tunes the interplay of electron, spin, orbital and lattice degrees of freedom characteristic of the transition-metal oxides. Oxygen vacancies (VOs) at the LAO/STO interface leave two vacant electrons, one of which stays localized at the Ti^{3+} ion and another joins the mobile 2DES. This forms a dichotomic electron system where the localized strongly correlated in-gap electrons coexist with the less correlated mobile ones. The localized electrons in double and higher-order configurations of the VOs may account for the interface ferromagnetism [1]. The mobile ones, coupled to phonon modes by strong electron-phonon interaction, form large multiphonon polarons fundamentally reducing the 2DES mobility [2]. The latter can however be tuned by the mobile electrons injected by the VOs which screen the electron- phonon interaction. The VOs are therefore an important piece of the reach LAO/STO physics in view of potential applications of oxide interfaces in electronics and spintronics.

We use resonant soft-X-ray ARPES experiments at the ADRESS beamline of Swiss Light Source to establish orbital character of the mobile and localized electron states at the LAO/STO interface created by the VOs. We identify the predominantly Ti e_g- vs t_{2g}-derived orbital character of these two electron systems. Furthermore, we distinguish different chemical states of the in-gap electrons, and demonstrate interface induced orbital selectivity of resonant photoemission allowing separation of the d_{xy}- vs $d_{xz/yz}$-derived bands of the mobile ones. DFT+DMFT calculations agree with the experiment on both energy position and orbital character of the localized and mobile electrons. In contrast to bare STO surface, where these electrons fall into purely e_g and t_{2g} character, at the LAO/STO interface these orbitals significantly hybridize. This finding of a crosstalk between the localized and mobile electron systems sheds new light of the mechanism of magnetism and superconductivity at the LAO/STO interface.

References:

[1] F. Lechermann, L. Boehnke, D. Grieger, and C. Piefke, *Physical Review B* **90 (8)**, 85125 (2014).
[2] C. Cancellieri, A. S. Mishchenko, U. Aschauer, A. Filippetti, C. Faber, O. S. Barišić, V. A. Rogalev, T. Schmitt, N. Nagaosa & V. N. Strocov, *Nature Communications* **7**, 10386 (2016).