Electronic Supplementary Information file for "Strain induced atomic structure at Ir-doped $LaAlO_3/SrTiO_3$ interface"

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Strain analysis in the LAO film

The relationship between ϵ^{GPA}, the strain measured in LAO by Fourier filtering processing (GPA method) relatively to the STO lattice, and ϵ, the elastic strain in LAO epitaxially grown on STO can be expressed by the following expression:

$$\begin{aligned} \epsilon_{\parallel}^{GPA} &= f + \epsilon_{\parallel} \times (a_{\mathrm{LAO}}/a_{\mathrm{STO}}) \approx f + \epsilon_{\parallel} \\ \epsilon_{\perp}^{GPA} &= f + \epsilon_{\perp} \times (a_{\mathrm{LAO}}/a_{\mathrm{STO}}) \approx f + \epsilon_{\perp} \end{aligned} \tag{1}$$

in which f represents the misfit parameter at the LAO/STO interface, $f = (a_{LAO} - a_{STO})/a_{STO} \approx$ - 3%. To fix the idea, one can expect $\epsilon_{\perp}^{GPA}$ to be close to -5.6 % in the non-doped case using the values of the misfit and of the strain components reported in equation (1) of the paper.

Figure SI-1 provides an example of the image processing used to determine the strain state in the LAO layer along directions parallel and perpendicular to the LAO/STO interface. It presents portions of an HAADF-STEM image and associated coloured maps of $\epsilon_{\parallel}^{\mathrm{GPA}}$ and $\epsilon_{\perp}^{\mathrm{GPA}}$. Strain values at each point of the image can then be extracted from such maps.

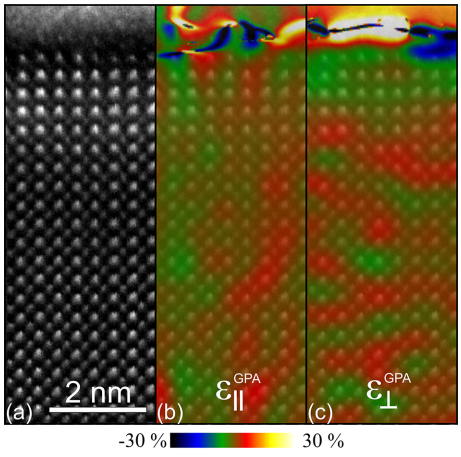


Figure SI-1: Strain analysis performed on a HAADF image using the GPA method. (a) HAADF image of the 1%Ir sample; (b) and (c) superimposed coloured maps of the $\epsilon_{\parallel}^{\mathrm{GPA}}$ and $\epsilon_{\perp}^{\mathrm{GPA}}$ respectively

Intermixing at interface

Figure SI-2 is given as a complement of Figure 4 in the paper.

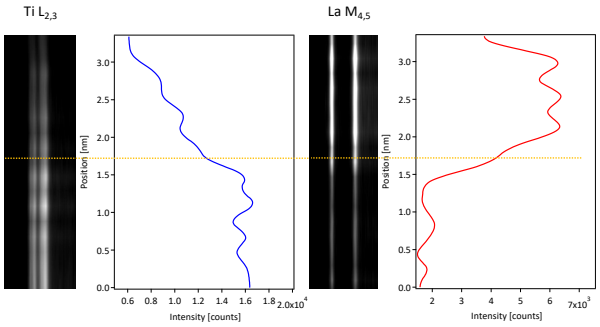


Figure SI-2: Intensities integrated under the EELS Ti-$L_{2,3}$ and La-$M_{4,5}$ edges recorded along the line scan displayed in Figure 4 of the paper

Details for DFT calculations

From the DOS plotted in the Fig. SI-4, we can clearly see the Ir gap states near the Fermi level, which are responsible of the shift of the Fermi level, and then of the EELS spectra. The A and B peaks are electronic states resulting respectively from the hybridization of orbitals from the oxygen and Ti atoms, and from the oxygen and Sr atoms. The nature of the C peaks is more difficult to analyse as the most important contribution comes from the interstitial region.

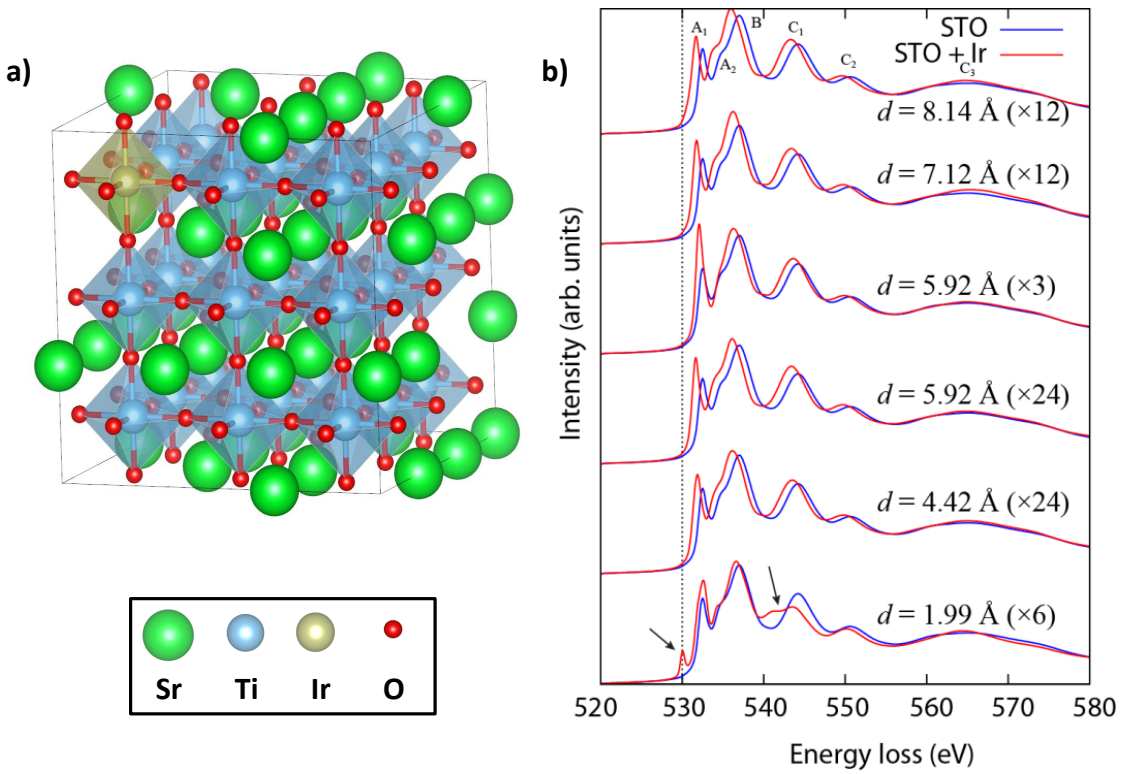


Figure SI-3: EEL spectra calculated for each non-equivalent oxygen atom present in the 3×3 Ir-doped STO supercell (red curves). These atoms are located at a distance d from the Ir impurity (and their multiplicity is given within the parentheses). The blue curves correspond to the EEL spectra calculated for non-doped STO and are plotted for comparison.

In the Fig. SI-5, we compare the EEL spectra calculated for both cubic and tetragonal LAO. For the tetragonal lattice, we fixed the lateral lattice parameters to those of the STO bulk: We can then distinguish two non-equivalent oxygen atoms, one located in the apex of the octahedra (with a multiplicity of 2) and the other one at the basis (with a multiplicity of 4). The red curve of the Fig. SI-5 corresponds to an average (taking into account of their multiplicity) of the spectra calculated for both non-equivalent oxygen atoms.

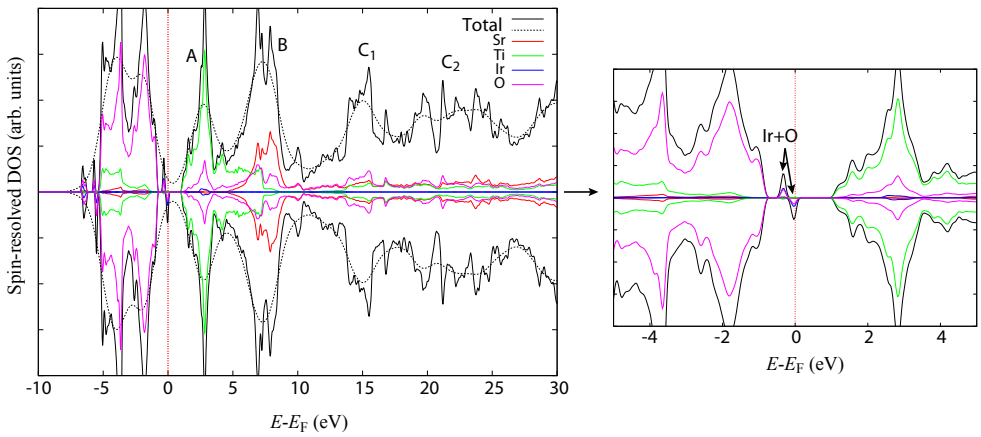
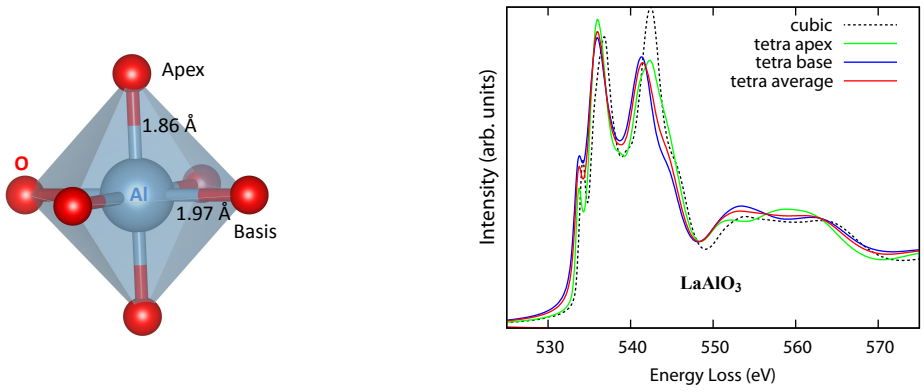


Figure SI-4: Spin-resolved density of states (DOS) with the majority and minority spin states represented respectively by the positive and negative curves. The total DOS is plotted with two different gaussian broadening for an easier comparison with the EEL spectra.



(a) (b)

Figure SI-5: a) Octrahedral chemical environment, b) EEL spectrum calculated for bulk cubic (black dotted line) and tetragonal (green, blue, red curves) LAO .