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# Supporting Information

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# Structural and Electronic Reconstructions at the $LaAlO_3/SrTiO_3$ Interface

*M. Salluzzo,* S. Gariglio, X. Torrelles, Z. Ristic, R. Di Capua, J. Drnec, M. Moretti Sala, G. Ghiringhelli, R. Felici, and N. B. Brookes*

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**Supporting information on the analysis of the Grazing Incidence x-ray diffraction data**

The structural models employed included the vertical displacements (perpendicular to the interface) of the A-site and B-site cations and of the oxygen ions in each $LaAlO_3$ and surface $SrTiO_3$ (001) layers. Additional parameters were the intermixing in the layers close to the interface, i.e. in the first LAO unit cells and the first three STO unit cells, and the La/Al occupancies at the LAO surface. This first model, model-1, considers full oxygen occupancy. A second model, model-2, includes as further refinement oxygen vacancies in the LAO film and in the first 4 unit cells in the STO layers. In **Figure S1** we show a comparison between the occupancies, z-displacements and rumpling of the planes obtained using the two models. The reduced $\chi 2$ $\chi^2 = \frac{1}{N-P}\sum\frac{\left(F_i^{Th}-F_i^{exp}\right)^2}{\sigma_i^2}$ obtained from a fit of the data on 2uc, 4uc and 6uc samples from Set-B are 0.55, 0.64 and 1.0 using model-1, and 0.52, 0.62 and 0.98 using model-2. For all the samples investigated, independent on the sample set and on the LAO thickness, the fit converged to solutions compatible with an oxygen-vacancy percentage around 2% in the first two STO layers (and in the LAO film). The displacements of the ions were only slightly modified by the introduction in the model of oxygen vacancies. In particular, the rumpling of the STO planes in our LAO/STO bilayers was mostly unchanged within the error bar [**Figure S1e**] and, as before, the oxygen ions displace towards the interface, while the A and B-site cations remain quite close to the ideal STO bulk positions.

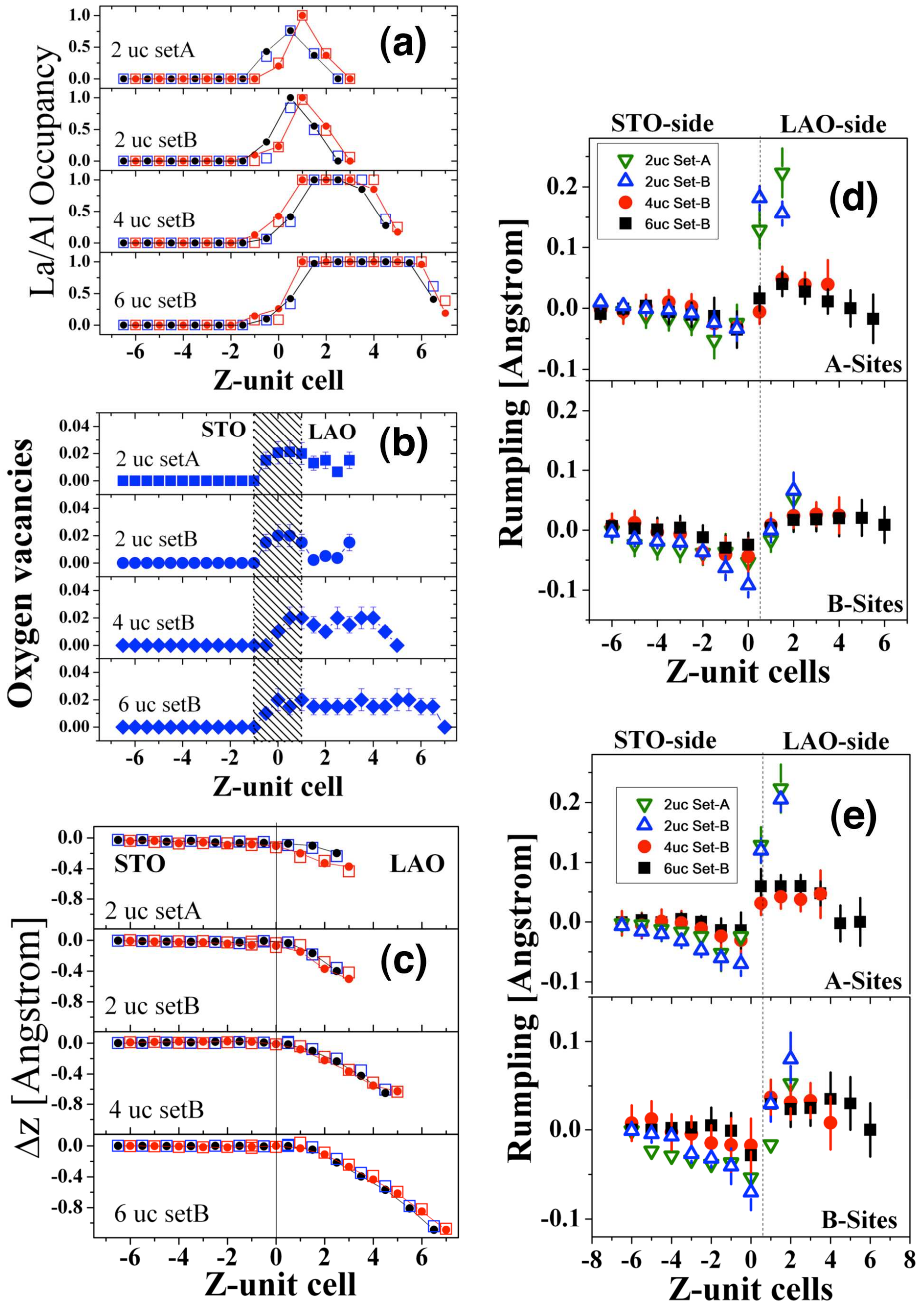


**Fig. S1**: (a) La/Al occupancies of the LAO/STO bilayers from structural refinement using two structural models: model-1, full oxygen occupancy (closed circles); model-2, oxygen vacancies model (open squares). Red (site-B) and black (site-A) closed circles are the result from model-1 (Figure 2 of the manuscript), while red (site-B) and blue (site-A) open squares are the occupancies obtained using model-2. (b) Corresponding oxygen vacancy level from model-2 for each sample as function of the layer-index. Dashed regions correspond to areas where cation intermixing is found from the refinement. (c) Cation displacements obtained from the refinement using the two models: red (site-B) and black (site-A) closed circles are the result from model-1 (Figure 2 of the manuscript), while red (site-B) and blue (site-A) open squares are the displacements obtained from model-2. Comparison between the rumpling of the AO and $BO_2$ planes obtained using model-1 (d) and model-2 (e).