Supporting information for 'Polarisation screening mechanisms at $La_{0.7}Sr_{0.3}MnO_3$-$PbTiO_3$ interfaces'

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1. DFT structure calculations

Figure S1 shows the structure of the $La_{0.7}Sr_{0.3}MnO_3$-$PbTiO_3$ (LSMO-PTO) interface determined from the DFT calculations. It is evident from Figs. S1(a) and S1(b) that the interface B-site displacement and octahedral tilt are different for the two polarisation directions (similar to Fig. 3 from the main text). Whilst the combination of high interface tilt with low interface displacement (and vice versa) is visible, these effects inversely correlate with the experimental observations in Fig. 3 in the main text. This is because of the different interface termination. Where Figs. S1(a) and S1(b) have a MnO_2 termination of the LSMO, the experimental observations are for a (La,Sr)O termination (Fig. 2(c) in the main text). Unfortunately, the DFT calculations for the (La,Sr)O structure with $P_{\downarrow}$ did not converge as the metal fermi level entered the ferroelectric conduction band due to the DFT band gap error (see experimental methods section in the main text). The results for the (La,Sr)O structure with $P_{\uparrow}$ are shown in Fig. S1(c) and S1(d), with the MnO_2 data overlaid (with the polar displacement values inverted). It stands to reason that, if the interface structure is determined by the LSMO charged interface, that inverting this charge (i.e. switching the interface termination) would invert the correlation with the polarisation direction. This is the case for the available DFT model, where the (La,Sr)O $P_{\uparrow}$ structure closely resembles the MnO_2 $P_{\downarrow}$ case.

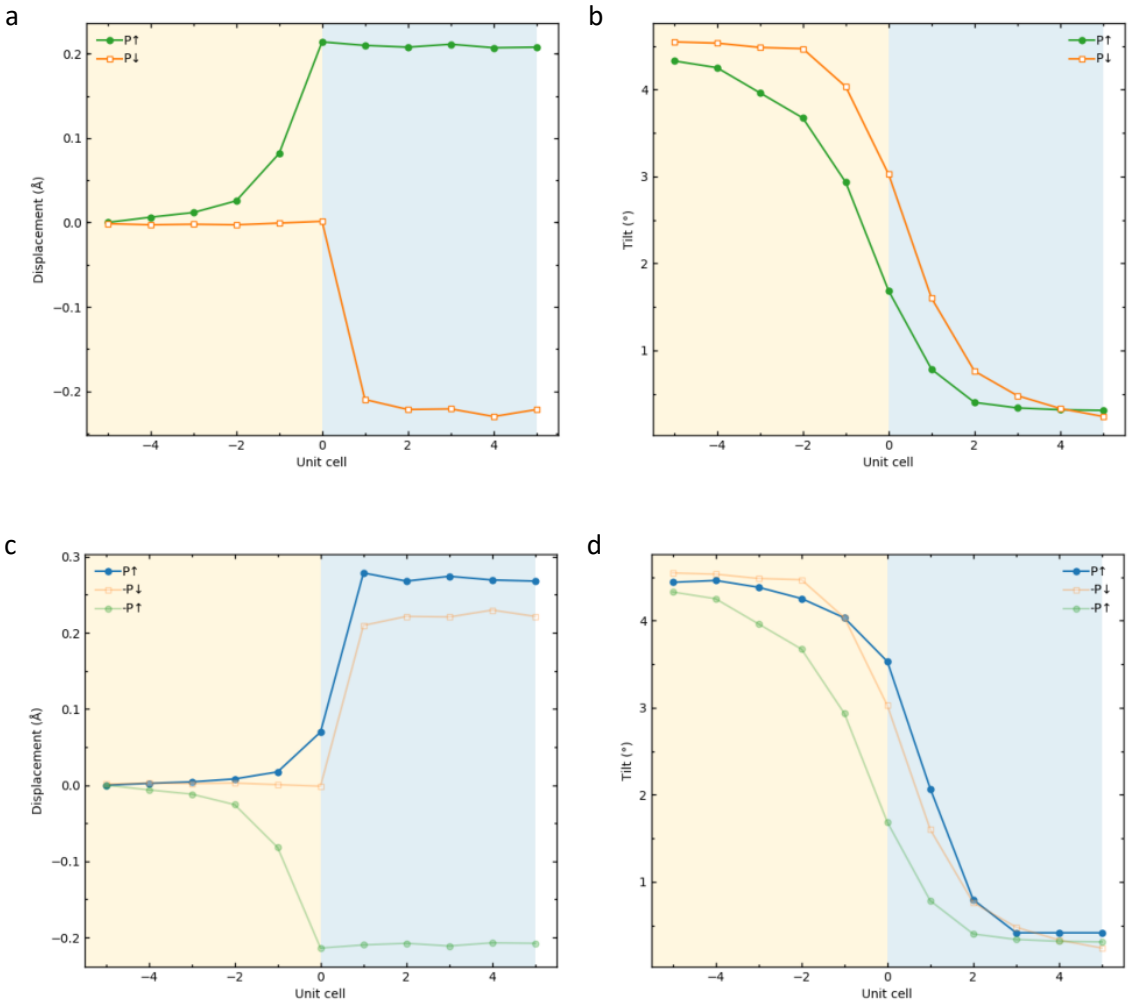

Figure S1 DFT calculations of the out of plane profiles for (a) B-site displacement (with respect to the oxygen octahedra) and (b) octahedral rotation for the MnO_2 interface termination. Data for both out of plane polarisations in presented. (c) B-site displacement and (d) octahedral rotation for the (La,Sr)O termination. Only data for polarisation up is shown, with the data for the MnO_2 interface overlaid (displacement values have been flipped to show similarities).