Supplementary Information: Wide gap Chern Mott insulating phases achieved by design

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Here we provide additional information on our study of the $(LaXO_3)_2/(LaAlO_3)_4$ (111) superlattices, X = Os and Ru. The X^{3+} ion has a $5d^5$ configuration, and the octahedral coordination splits the e_g states well above t_{2g}. The trigonal crystalline field arising from the (111) growth will split the threefold t_{2g} into $e'_g + a_{1g}$, and the symmetric expression adapted to trigonal symmetry for t_{2g} orbitals is

$$|\Psi_m\rangle = i\frac{1}{\sqrt{3}}(\zeta^0_m|d_{xy}\rangle + \zeta^0_m|d_{yz}\rangle + \zeta^2_m|d_{xz}\rangle) \qquad (1)$$

where $\zeta_m = e^{2\pi i m/3}$. $m = \pm 1$ represent the e'_g orbitals, $m = 0$ is the a_{1g} orbital. Also m is the orbital magnetic quantum number. For the t_{2g} subshell the dominating feature is a competition between local pseudo-cubic symmetry and the underlying threefold and inversion symmetry (P321) of the ideal layer. Relaxation to $P1$ symmetry mixes the Ψ_m orbitals, and will mix in some e_g character in an amount depending on the crystal field splitting.

Considering 2 X atoms, 3 orbitals and 2 spins, 12 t_{2g} bands are involved. Due to the d^5 configuration, two t_{2g} bands ("one per metal ion") will be unoccupied. When time reversal symmetry is broken, and the repulsive interaction U and the SOC are both included, a topologically Chern insulating phase may be realized.

Osmate. The SOC effect on the d-projected density of states (pDOS) of both Os1 and Os2 sites in 2LOsO is shown in Fig. 1. The upper four panels are for a_{LAO}, the bilayer that is a Chern insulator with $C = +2$. There are very few differences between the pDOS of Os1 and Os2, consistent with the minor distortion during the relaxation from P321 to P1 as mentioned in the main text. Without SOC, a narrow peak overlaps Fermi level, which corresponds to a flat band region. In the trigonal coordinate system, the d_{z^2} orbital is a_{1g} character, the rest can be considered to be e'_g character. The narrow peak is mixed a_{1g} and e'_g character. SOC splits this peak, opening a 46 meV gap corresponding to the band anticrossing occurring near the Fermi level, see Fig. 4 in the main text. As a consequence of this entanglement by anticrossing, a Chern insulating phase is obtained.

The lower four panels are the analogous plots for a_{LNO}. Here the pDOS of Os1 is much different than that of Os2, which is attributed to the large distortion and symmetry reduction resulting from the strain. The dominant character, the pDOS weight, and the band width of the valence bands are different for the two Os sites. Compared to those for a_{LAO}, there are no flat band regions, and the gap is already opened before SOC is applied. SOC slightly reduces the gap, and the effect of all the differences is to leave a trivial insulating phase.

Ruthenate. Fig. 2 shows the analogous d pDOS of Ru sites in the 2LRuO bilayer. The upper four panels are for a_{LAO}, which is a trivial insulator; the lower four are for a_{LNO}, which is Chern insulator with $\mathcal{C}$=-1. Again for the Chern insulating phase, the Ru1 and Ru2 sites are almost equivalent in their electronic structure. For trivial insulating phase, however, the Ru1 and Ru2 sites have differing d electronic structures. The narrow peak which reflects the flat band region near the Fermi level exists for both lattice constants;, that of Ru@a_{LAO} is dominated by d_{xy} electrons, while that of Ru@a_{LNO} also has a_{1g} character – the same situation as for the Chern insulating 2LOsO bilayer. Notably, for Ru@a_{LNO}, the narrow peak before SOC splits and opens a 132 meV gap, which combined with band anticrossing produces the Chern insulating phase. Both Chern insulating bilayers have holes primarily of a_{1g} character.

Energy-resolved Chern number. The energy-resolved (*i.e.* variable chemical potential) Chern number is provided in Fig. 3. It is apparent that the coefficient of e^2/h accurately attains the integer $\mathcal{C} = 2$ value for 2LOsO across the 46 meV gap, and attains $\mathcal{C}$=-1 for 2LRuO over its 132 meV gap.

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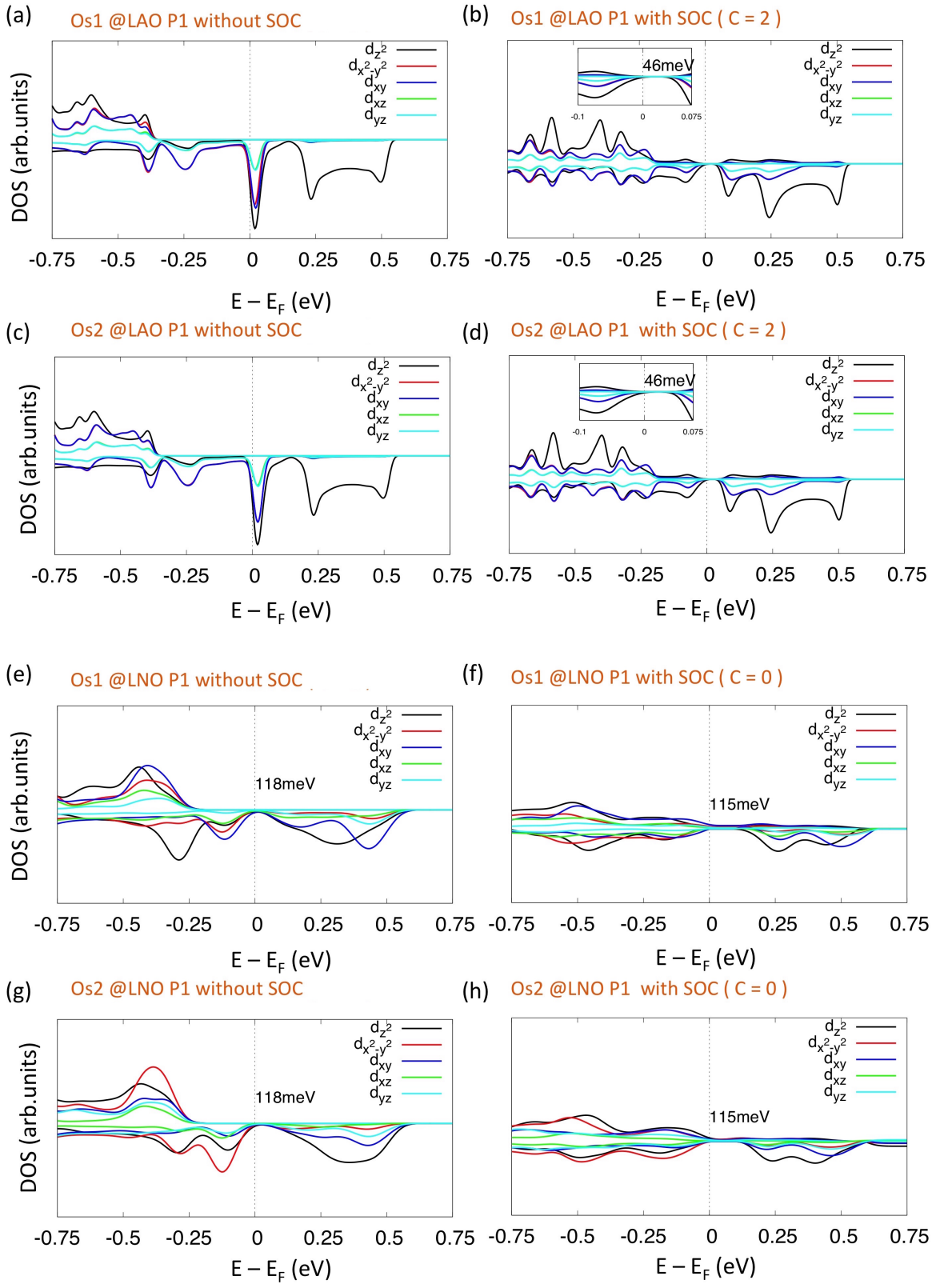

FIG. 1. The d projected density of states of the two inequivalent Os atoms in 2LOsO bilayers with P1 symmetry.The left panels, before including SOC; right panels, with SOC included. Upper four panels(a,b,c,d): pDOS of the two Os in 2LOsO bilayers corresponding to lattice constant a_{LAO}; lower four panels (e,f,g,h): analogous plots for a_{LNO}.

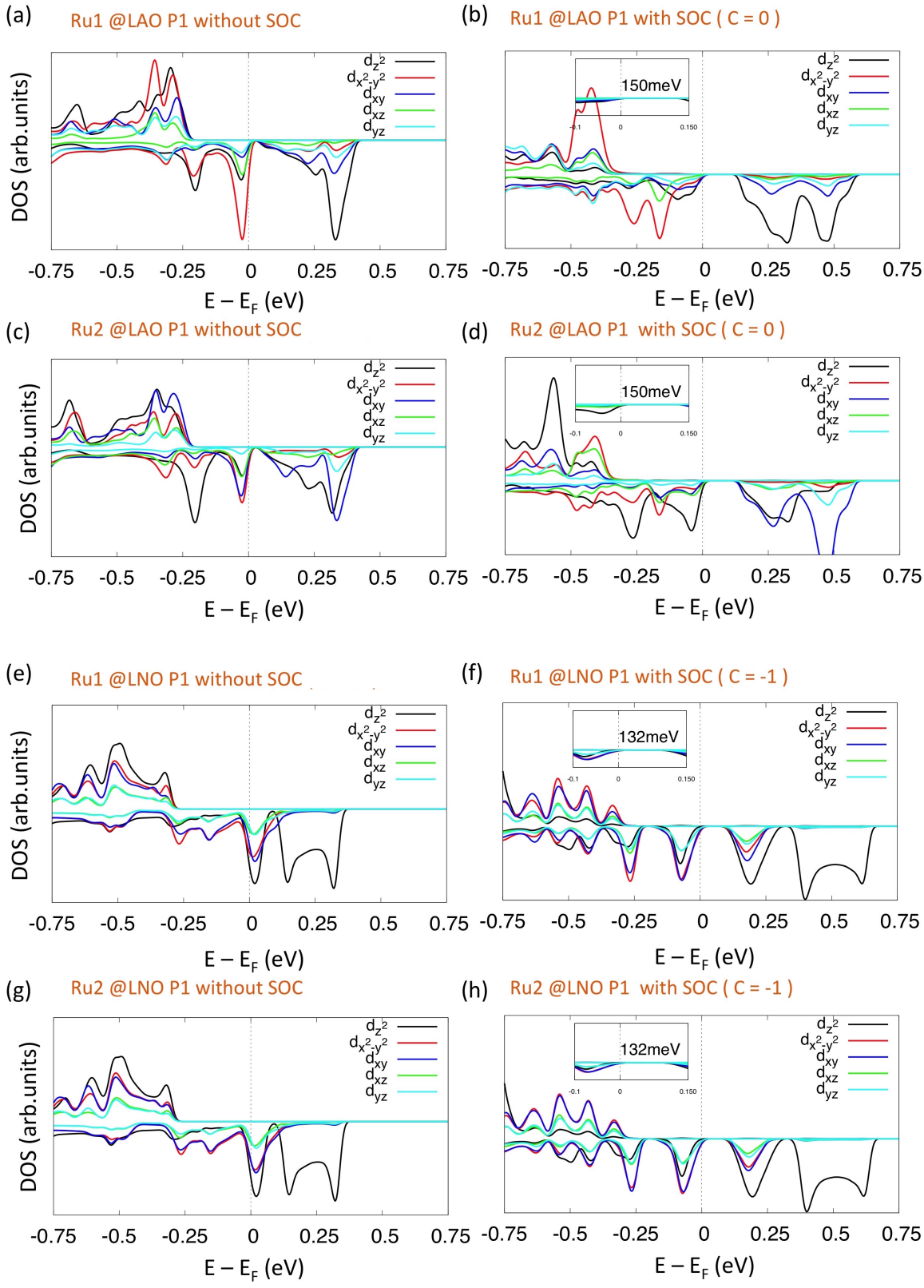

FIG. 2. As for Fig. 1, but for 2LRuO.

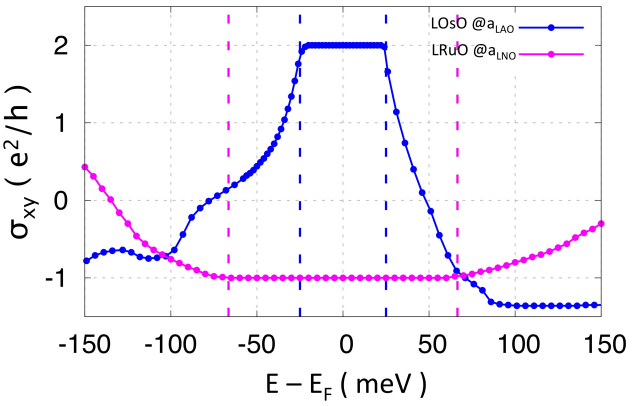

FIG. 3. The calculated anomalous Hall conductivity σ_{xy}, plotted in units of e^2/h versus the chemical potential. Curves for both of the Chern insulator states are shown. The flat region indicates the gap, whose edges are given by dashed vertical lines. The relative positioning of the two curves is irrelevant.