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Landau theory of topological defects in multiferroic hexagonal manganites

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I. FIRST-PRINCIPLES CALCULATIONS

FIG. S1: Left panel: Phonon band structure of the high-symmetry phase (P6₃/mmc) of YMnO₃, obtained using frozen-phonon methods and Fourier interpolation of the interatomic force constants. The most unstable zone-boundary mode at K is the K_3 trimerisation mode. Right panel: Extraction of the s_Q^x stiffness parameter by fitting the dispersion of the force constant of the trimerisation mode.

II. MAGNETIC FREE ENERGY

The estimates for some coefficients in the expression for the magnetic free energy Eq.(3)(per 1 f.u.) can be obtained using the parameters of the spin Hamiltonian extracted from the magnon spectra of YMnO₃^{S1}: $S = 22$ meV·Å², $A = -0.003$ meV, $C_+ = -0.076$ meV. A more detailed information is provided by the recent first-principles study of magnetic structures of YMnO₃ and LuMnO₃.^{S2} Using the energies of the $A_{1,2}$ and $B_{1,2}$ states and the exchange constants calculated in that work we obtain the coefficients shown in Table SI. The magnetisation M_{A_2} due to canting of Mn spins in the A_2 state is $1.4 \times 10^{-2} \mu_B$ per Mn ion, for both materials.

The magnetic structure of the domain walls shown in Fig. 4 was calculated assuming that

	$S(\text{meV}\cdot\text{\AA}^2)$	$A(\text{meV})$	$C_+(\text{meV})$	$C_-(\text{meV})$
YMnO ₃	58	-0.11	0.08	0.00
LuMnO ₃	56	0.07	0.24	0.00

TABLE SI: Parameters of the phenomenological expansion of the magnetic free energy Eq. (3) per 1 f.u.

the B_2 state has the lowest free energy (using LuMnO₃ parameters).

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