sample plates and mounted on the cold finger of a helium flow cryostat. Prior to the measurements, each sample was mechanically cleaved in the fast-entry chamber at a pressure of $\sim 10^{-9}$ mbar to expose a pristine surface. The sample was then transferred into the spectroscopy chamber with a pressure in the 10^{-11} – 10^{-10} mbar range.

The measurements were carried out in the TEY or FY mode at magnetic fields of up to 6 T and at various temperatures in the 3.5–35 K range. The temperature was calibrated with a thermal sensor mounted at the sample position before the experiment. Especially below about 5 K, the actual sample temperature crucially depends on the thermal contact, increasing its error as compared to higher temperatures. The spectral intensity was normalized by the incoming photon intensity (I_0). We used circularly polarized light at both beamlines. The area probed by the beam at both facilities (about $120\times80\mu\mathrm{m}^2$) was much smaller than the sample size.

The raw XAS spectra were scaled with respect to each other to have the same intensity at energies far from the resonances to obtain I_{left} and I_{right}. We define the XMCD signal as $I_{\mathrm{XMCD}} = I_{\mathrm{left}} - I_{\mathrm{right}}$. The average, not background corrected XAS is $I = (I_{\mathrm{left}} + I_{\mathrm{right}})/2$. To cancel out any experimental drifts, for each data set we measured eight spectra in a row by altering the X-ray polarization. Finally, the magnetic moments measured with XMCD are marked with the subscript XM, e. g. $m^{\mathrm{tot}}_{\mathrm{XM}}$.

E. MLFT calculations

As a starting point to obtain input parameters for the MLFT modeling, self-consistent DFT in the linear density approximation is sufficient, which we performed using the FPLO package [81]. The Brillouin zone was sampled by a $2 \times 2 \times 2$ k-point mesh. The exchange-correlation potential was treated in LDA, with the scalar relativistic functional according to Ref. 82. We have used the experimental crystal structure from Ref. 31: rhombohedral space group $R\bar{3}m$ (166), $a = 4.37$ Å and $c = 101.83$ Å, slightly distorted octahedral Mn coordination with Mn-Te bond length of 3.00 Å (C_{3v} crystal field symmetry). We obtained Wannier orbitals as input for MLFT by downfolding to a basis set of Mn $3d$, Te $5p$ and Bi $6p$ orbitals in an energy window from -6 to 3 eV including an exponential decaying tail with a decay of 1 eV at the boundaries of the selected energy range.

The MLFT calculations were performed using the Quanty package [44, 83, 84] within the CI scheme considering the nominal $2p^6 3d^5$ (Mn^{2+}) configuration and two further charge-transfer states $d^6\underline{L}$ and $d^7\underline{L}^2$. The spectral contributions from the split ground-state terms were weighted by a Boltzmann factor for $T = 2\,\mathrm{K}$. The mean-field effective potential was modeled by an exchange field estimated from the T_{c} of 12 K. Instrumental and lifetime effects were taken into account by a Gaussian broadening of 0.35 eV (FWHM) and an E-dependent Lorentzian profile of $0.15 - 0.35\,\mathrm{eV}$ (FWHM).

The Slater integrals for the MLFT calculations were obtained by DFT, where $F^{(2)}_{dd}$ and $F^{(4)}_{dd}$ were scaled up by 8% for the final state, improving the agreement to experiment. SO coupling constants were kept to the Hartree-Fock values [47]. $\Delta = E(d^{n+1}\underline{L}) - E(d^n)$, U_{dd} and U_{pd} were directly fitted to the experimental spectra, keeping $U_{dd}/U_{pd} = 0.8$ [85–88]. Experiments involving charge-neutral excitations such as XAS are only weakly sensitive to Δ, U_{dd} and U_{pd}. In our particular case we were fitting simultaneously XAS and XMCD spectra, which substantially mitigates these kind of problems. Our results are in good agreement with values reported for (Ga,Mn)As [89–93] and Mn-doped Bi_2Se_3 [55] and Bi_2Te_3 [94]. The other MLFT input parameters were estimated from DFT, and their values were subsequently adjusted to reproduce the experimental spectra. To simplify the calculation, instead of the trigonal C_{3v} we work in O_h symmetry, with the C_4 octahedral axes along the Mn-Te bonds, which has a negligible impact: Our simplification neglects the splitting of the t_{2g} orbitals, which is tiny compared to $10Dq < 100\,\mathrm{meV}$, which in turn is smaller than the experimental resolution.

F. XMCD Sum Rule and Peak Asymmetry Analysis

The XMCD sum rules yield:

$$m^{\mathrm{orb}}_{\mathrm{XM}} = -\frac{4}{3}\frac{q}{r}(10 - n_d), \tag{1}$$

$$m^{\mathrm{spin}}_{\mathrm{XM}} = -\frac{6p - 4q}{r}(10 - n_d)C + 7\langle T_z\rangle, \tag{2}$$

where p and q are the XAS intensity differences ($I_{\mathrm{left}} - I_{\mathrm{right}}$) integrated over the L_3 edge and the entire $L_{2,3}$ region, respectively (Fig. 6). The XAS intensity I, after background correction (sec. S.V-A), is integrated over $L_{2,3}$ to yield r. $\langle T_z\rangle$ is the expectation value of the intra-atomic magnetic dipole operator which is $-0.0002\hbar$ and hence negligible (sec. S.V-A). For n_d we use the MLFT value of 5.31 (sec. II E). Finally, C is a correction factor, which takes into account the considerable overlap of the L_3 and L_2 contributions for light transition metals. We use a value of $C = 1.4$ (sec. S.V-A). To circumvent the difficulties related to this overlap, one can obtain $m^{\mathrm{spin}}_{\mathrm{XM}}$ by a comparison of the experimental XMCD asymmetry at the L_3 peak to the theoretical one calculated from MLFT spectra of comparable line width [52–54].

V. AUTHORS CONTRIBUTIONS

L.F., E.K. and A.I. conducted and analyzed the experimental work related to crystal growth, XRD and