Electronic Supplementary Information (ESI) for

Exploring the Effect of Intercluster Torsion Stress on Mn$^{2+}$-Related Emission from Cluster-Based Layered Metal Chalcogenides

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Figure S1. PXRD patterns of F-T4-Zn (a), T-T4-Zn (b), F-T4-Mn (c), and T-T4-Mn (d).

Figure S2. TGA curves of F-T4-Zn (a), T-T4-Zn (b), F-T4-Mn (c) and T-T4-Mn (d). The weight loss of 20.01 % for T-T4-Zn between 200-610 °C could be attributed to the loss of the charge-balanced DMP and AEP molecules (Calcd. 20.99%). For T-T4-Zn, about 24.48% weight loss was observed from 200°C to 400 °C, which is attributed to the removal of DMP molecules (Calcd. 25.07%). F-T4-Mn undergoes the weight loss about 22.92% from 200°C to 400 °C, corresponding to the removal of TAEA molecules (Calcd. 21.31 %). An abrupt weight loss of 24.18% in T-T4-Mn between 200-400 °C is attributed to the carbonization of the DMP molecules (Calcd. 25.44 %).
**Figure S3.** Energy dispersive X-ray spectroscopy (EDS) of F-T4-Zn (left) and T-T4-Zn (right). The insets are SEM images of the as-synthesized crystals.

**Figure S4.** Energy dispersive X-ray spectroscopy (EDS) of F-T4-Mn (left) and T-T4-Mn (right). The insets are SEM images of the as-synthesized crystals.

**Figure S5.** Low-temperature PL spectra of T-T4-Zn.
Figure S6. 2D PLE and PL spectra of the F-T4-Zn (a); F-T4-Mn (b) and T-T4-Mn (c).

Figure S7. PL quantum yield for F-T4-Mn.
Figure S8. PL quantum yield for T-T4-Mn.

Figure S9. PL quantum yield for F-T4-Zn.

Figure S10. The room-temperature PL decay curves of F-T4-Zn.
Figure S11. The crystal unit cell parameters of F-T4-Mn and T-T4-Mn at different temperature.

Scheme S1. The structure of template molecules used in this work.
Table S1. Structure refinement parameters on OCF-98-ZnInS, OCF-98-MnInS, OCF-99-ZnInS and OCF-99-MnInS.

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Table S2. The selected bond lengths (Å) for F-T4-Zn, T-T4-Zn and F-T4-Mn.

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### T-T4-Zn

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Symmetry: 1, 1-X, 1/2+Y, 1/2-Z; 2, +X, 1/2-Y, -1/2+Z.
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Symmetry: 1, -X, 1/2+Y, 1/2-Z; 2, +X, 1/2-Y, -1/2+Z; 3, 1-X, -1/2+Y, 1/2-Z; 4, +X, 1/2-Y, 1/2+Z.
Table S4. PL lifetime of F-T4-Zn, F-T4-Mn and T-T4-Mn at room temperature.

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Table S5. The crystal unit cell parameters for F-T4-Mn and T-T4-Mn at different temperature.

**F-T4-MnInS**

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**T-T4-MnInS**

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