Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Local structure and controllable thermal expansion in the solid solution $(Mn_{1-x}Ni_x)ZrF_6$

Fei Han,[1] Lei Hu,[1] Zhanning Liu,[1] Qiang Li,[1] Tao Wang,[1] Yang Ren,[2] Jinxia Deng,[1]Jun Chen, [1, †] and Xianran Xing[1]

[1]Department of Physical Chemistry, University of Science and Technology Beijing, Beijing 100083, China

[2]Argonne National Laboratory, X-Ray Science Division, Argonne, Illinois 60439, USA

[†]Corresponding Author, Electronic mail: Junchen@ustb.edu.cn

Result and Discussion

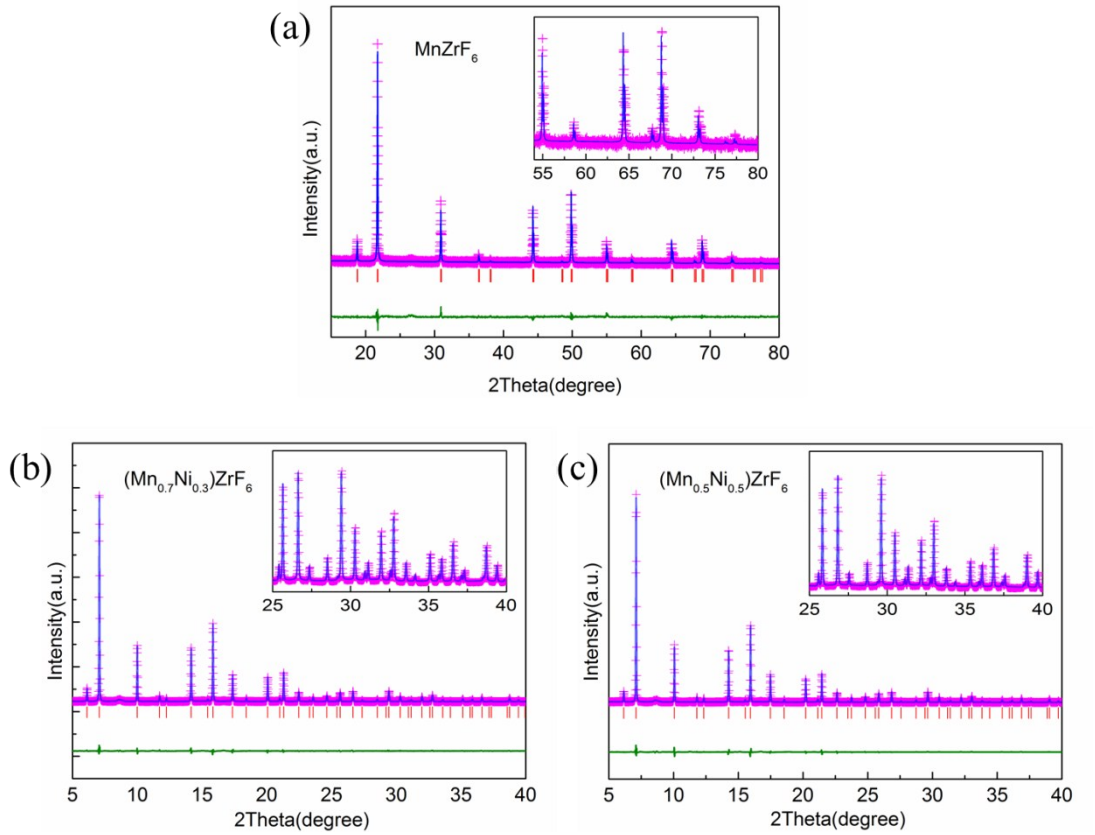

Figure S1. XRD patterns obtained from a laboratory diffractometer for (a) $MnZrF_6$ and High-resolution SXRD patterns for (b) $(Mn_{0.7}Ni_{0.3})ZrF_6$ and (c) $(Mn_{0.5}Ni_{0.5})ZrF_6$. The observed and calculated diffraction data are signed by purple crosses and blue line, respectively. The green lines and red bars in the lower part of patterns show the difference and peak positions, respectively. The high angular is enlarged and exhibited in the insets.

Table S1. Lattice constants of $(Mn_{1-x}Ni_x)ZrF_6$ (x = 0, 0.3, 0.4, 0.8) for various temperatures

Temperature /K	$MnZrF_6$	$(Mn_{0.7}Ni_{0.3})ZrF_6$	$(Mn_{0.6}Ni_{0.4})ZrF_6$	$(Mn_{0.2}Ni_{0.8})ZrF_6$
300	8.17653	8.12065	8.08871	7.99509
350	8.17363	8.11990	8.08950	7.99752
400	8.17156	8.11921	8.08936	7.99911
450	8.16942	8.11757	8.08931	8.00066
500	8.16765	8.11709	8.08891	8.00120
550	8.16611	8.11617	8.08886	8.00198
600	8.16490	8.11553	8.08905	8.00296
650	8.16340	8.11531	8.08963	8.00437
700	8.16226	8.11505	8.0898	8.00592

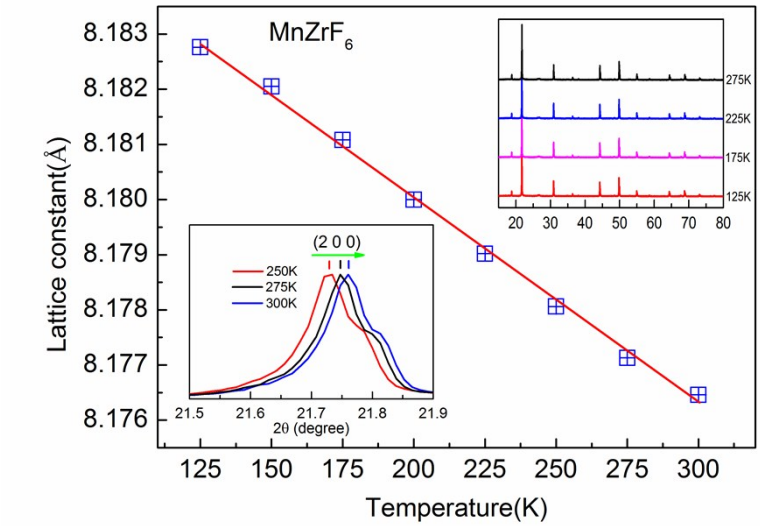

Figure S2. Temperature-dependence lattice constant of $MnZrF_6$ in the low temperature region. The inset at the top-right displays the XRD patterns at the investigated temperatures, indicating no phase transition occurs. The panel at the left-bottom shows the variation of (2 0 0) peak from 250 to 300 K.

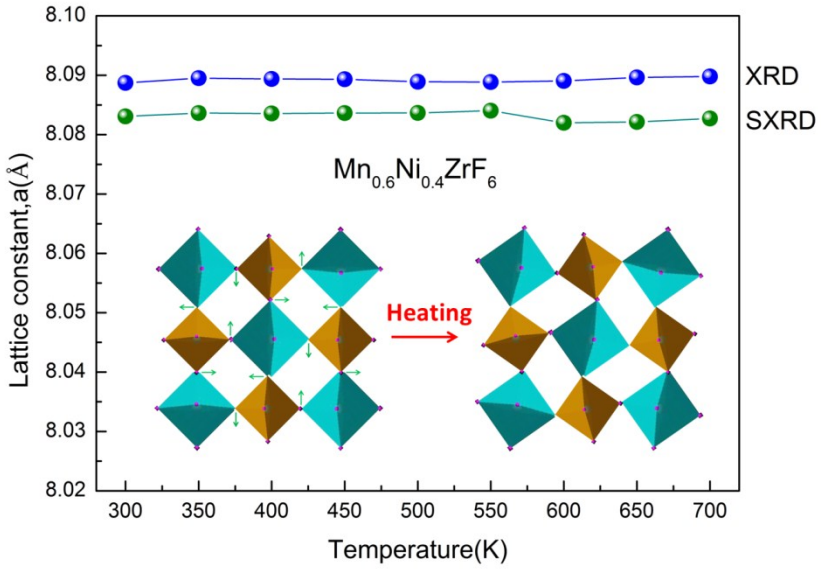

Figure S3. Temperature evolution of lattice constant of $(Mn_{0.6}Ni_{0.4})ZrF_6$ measured in two ways to confirm the reliability of ZTE property. The bottom region exhibits the vibration mode upon heating

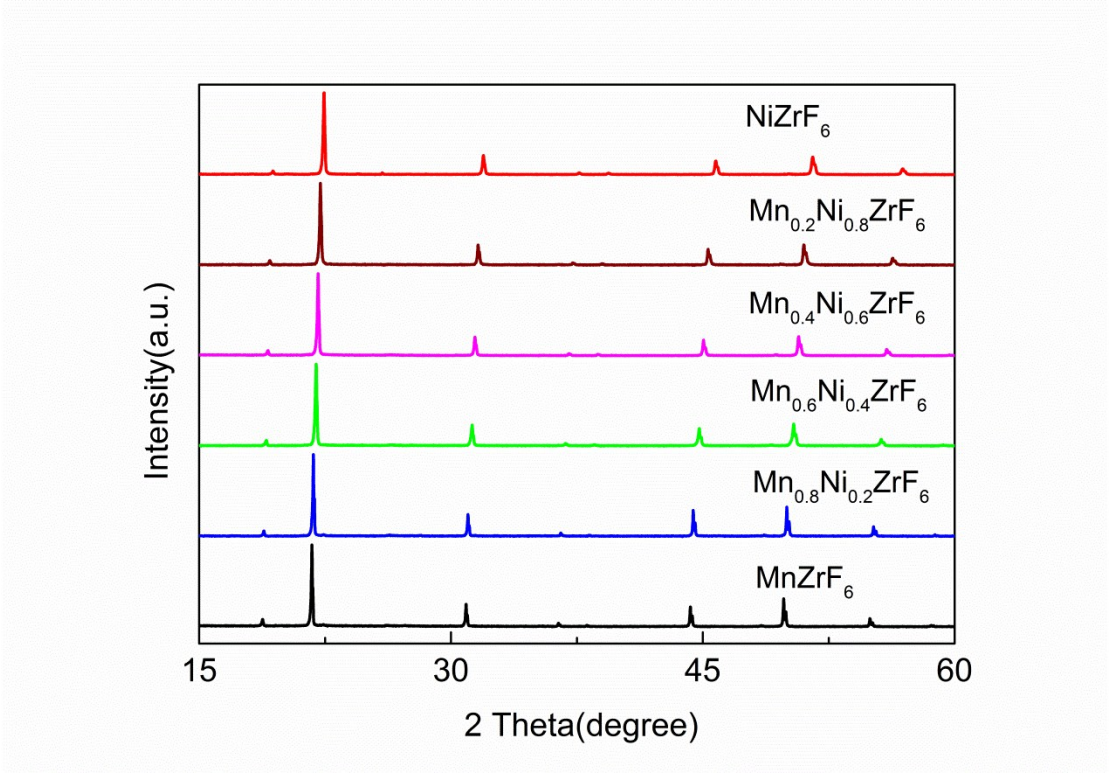

Figure S4. XRD patterns of $(Mn_{1-x}Ni_x)ZrF_6$ as a function of *x*.

Table S2. The slope of apparent bond length for *M*-F and Zr-F linkages

Compound	M-F ($k\times10^{-6}$)	Zr-F ($k\times10^{-6}$)
$MnZrF_6$	6.0	-42.3
$Mn_{0.6}Ni_{0.4}ZrF_6$	12.1	-8.3
$NiZrF_6$	28.4	36.3