Supplementary Information

Emergence of heavy-fermion behavior and distorted square nets in partially vacancy-ordered $Y_4Fe_xGe_8$ ($1.0 \leq x \leq 1.5$)

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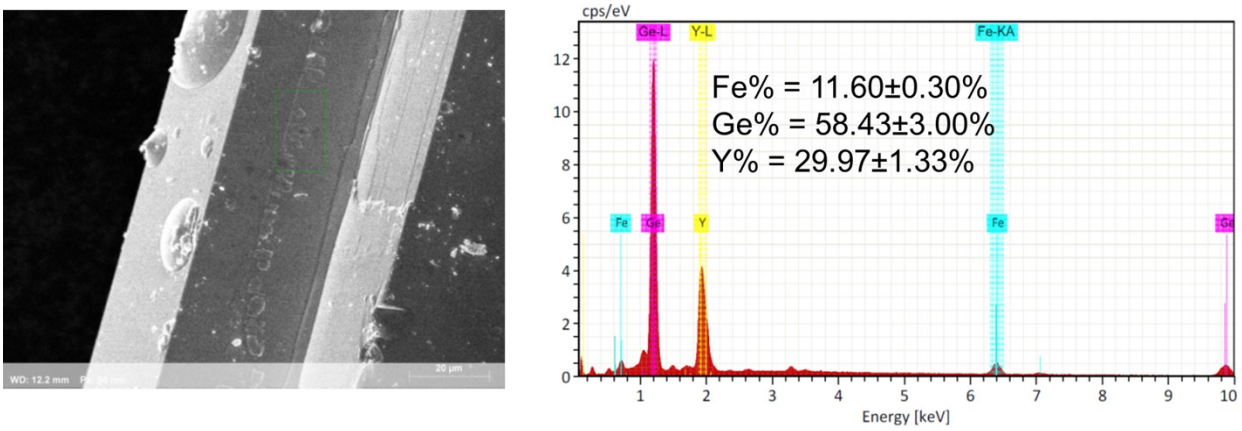

Figure S1. Elemental analysis for sample $Y_4Fe_xGe_8$ using EDS. It gives a Y:Fe:Ge ratio of about 4:1.5:8, very close to our single crystal refinement (x = 1.44) as shown in **Table 1**.

Symmetry and space group evolutions

The $CeNiSi_2$-type structure, which crystallizes in the orthorhombic *Cmcm* space group, restricts both the Ge-Ge square net to be perfect and the Fe-site to be centered (**Fig.S2a**). As observed in the Tb_4FeGe_8,[1] with only the Ge square-net distortion enabled, the Ge square-net distorts from rhombi to irregular quadrilaterals resulting in four distinct Ge-Ge distances for each Ge, breaking all mirror and glide planes of the space group *Cmcm* and thus lowering the symmetry down to monoclinic space group $P2_1/n$ (**Fig.S2b**). Note the Fe-site is still centered under this symmetry (**Fig.S2b**). By further allowing the Fe-site to move off-centered, as we have observed in the titled compound as well as in the Y_4RuGe_8,[2] the symmetry get further reduced down to triclinic space group *P-1* (**Fig.S2c**).

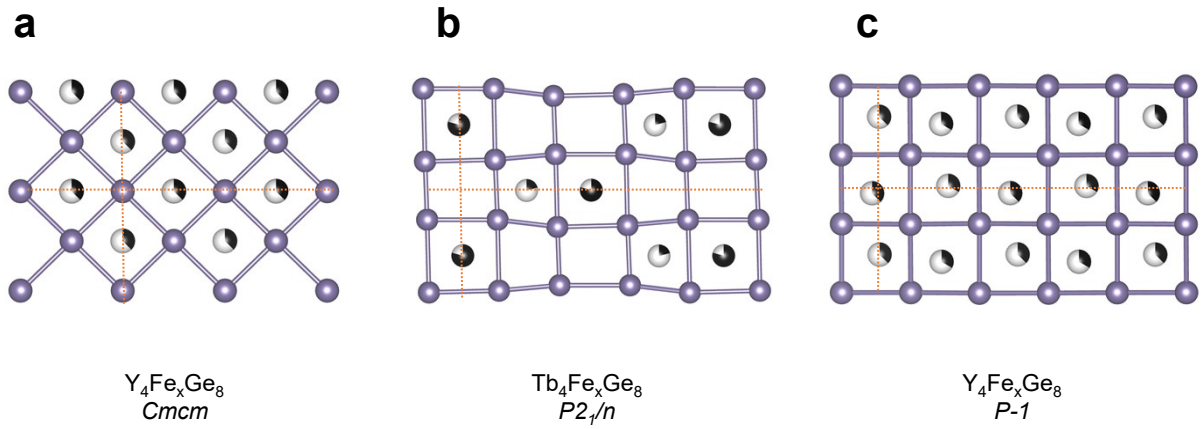

Figure S2. Schematic of the evolution of space group as a result of both Ge-Ge square net distortions and the Fe-site off-centering, with **a)** $Y_4Fe_xGe_8$, Orthorhombic space group *Cmcm*; **b)** Tb_4FeGe_8, monoclinic, space group $P2_1/n$ and **c)** $Y_4Fe_xGe_8$, triclinic space group *P-1*.

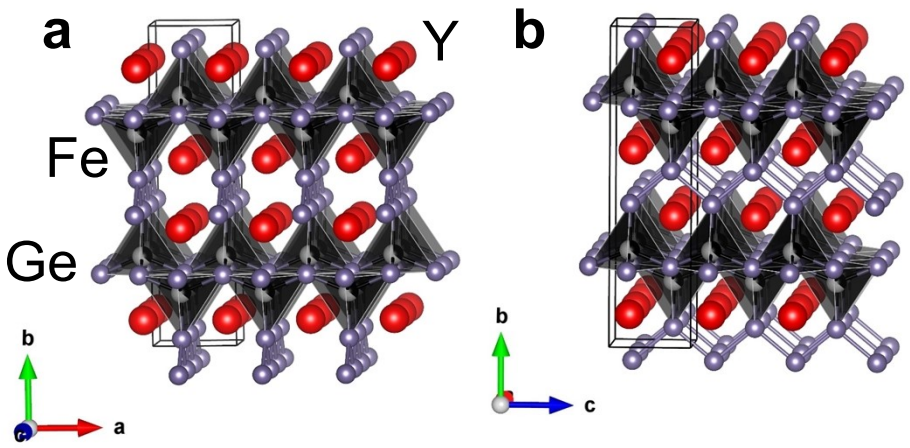

Figure S3. Crystal structures of $Y_4Fe_xGe_8$, crystallizing in a $CeNiSi_2$–type structure (*Cmcm* space group) viewing at **a**) the *ab*-plane and **b**) the *bc*-plane with $FeGe_4$ tetrahedron.

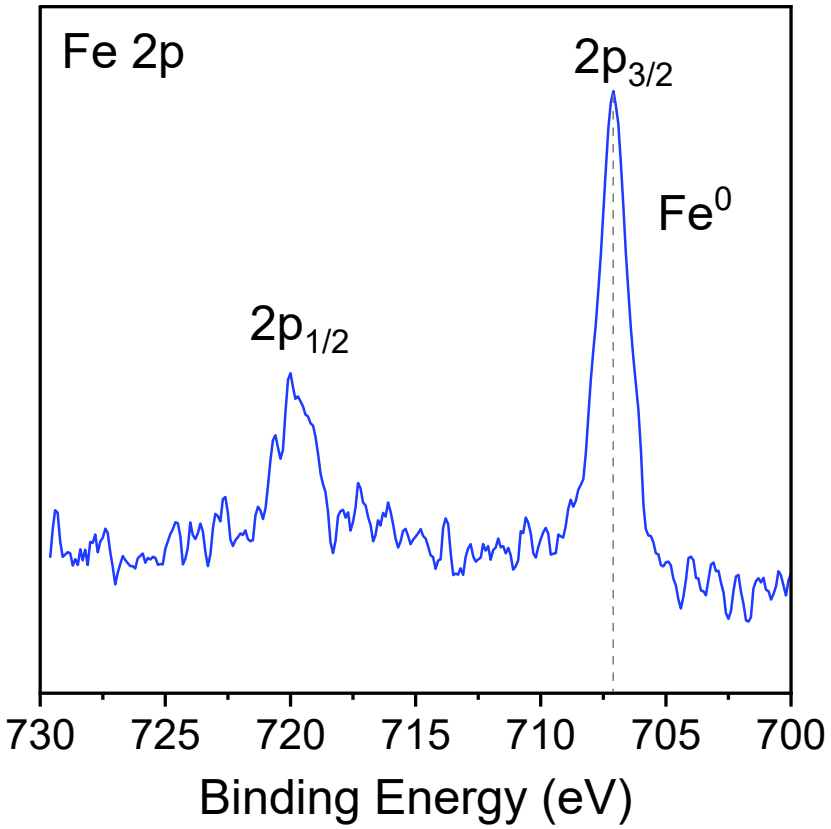

Figure S4. X-ray photoelectron spectroscopy (XPS) measurements of $Y_4Fe_{1.44}Ge_8$

Photoemission yield spectroscopy in air

PYSA measurements were taken on a Riken-Keiki AC-2 spectrometer. Thin film samples were scanned by tunable monochromatic ultraviolet light (UV, 4.2-6.2 eV) under dry air, and emitted photoelectron counts were measured at each excitation energy using an accelerating voltage of 2980 V with a counting time of ten seconds and a step size of 0.1 eV. A detector dead-time of

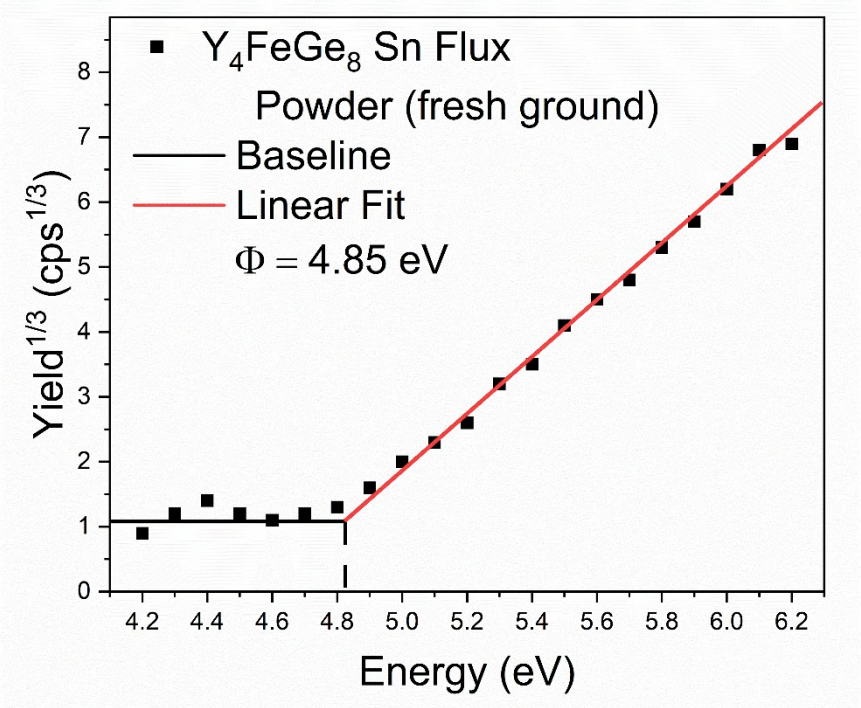

Figure S5. Photoemission yield spectroscopy in air (PYSA) measurements of $Y_4Fe_xGe_8$ performed with freshly ground powder.

5.6 ms was used, allowing a maximum counting rate of 1785/s. Maximum signal-to-noise ratio was obtained by setting the UV intensity to 300 nW for crystals and 200 nW for power, and a quantity-of-light correction was used to account for variations in UV lamp intensity across the energy range. First ionization energies of $Y_4Fe_xGe_8$ samples were determined by plotting the third root of photoelectron count rate against excitation energy, and a linear regression was used to determine the onset energy of above-baseline photoelectron flux. The negative of this onset energy was used as an approximation of the energetic position of the valence band maximum in the sample.

PYSA measurements performed on single crystals had apparent ionization energy of 5.47 eV, but freshly ground powder showed a shallower ionization energy of 4.85 eV. Re-measuring the same powder sample after 5 days in air yielded an apparent ionization energy of 5.11 eV. These values are consistent with surface oxidization of the starting crystals and the air-exposed powder. However, the ionization energy of the freshly ground powder (4.85 eV) is likely the closest approximation of the true work function of Y4FeGe8.

Magnetic Susceptibility Data for $Y_4Fe_xGe_8$ samples synthesized via Direct-Combination Method

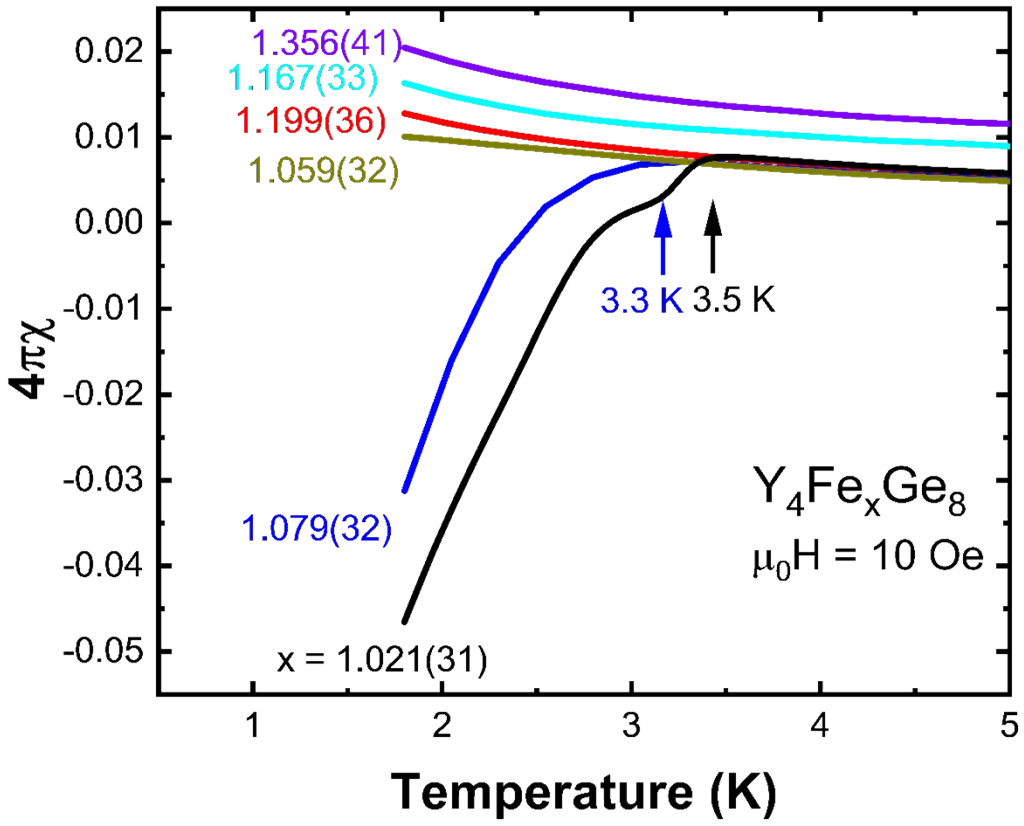

Figure S6. Zero-Field-Cooled (ZFC) volume magnetic susceptibility of selected Y4FexGe8 synthesized via direct-combination method with no indium/tin involved.

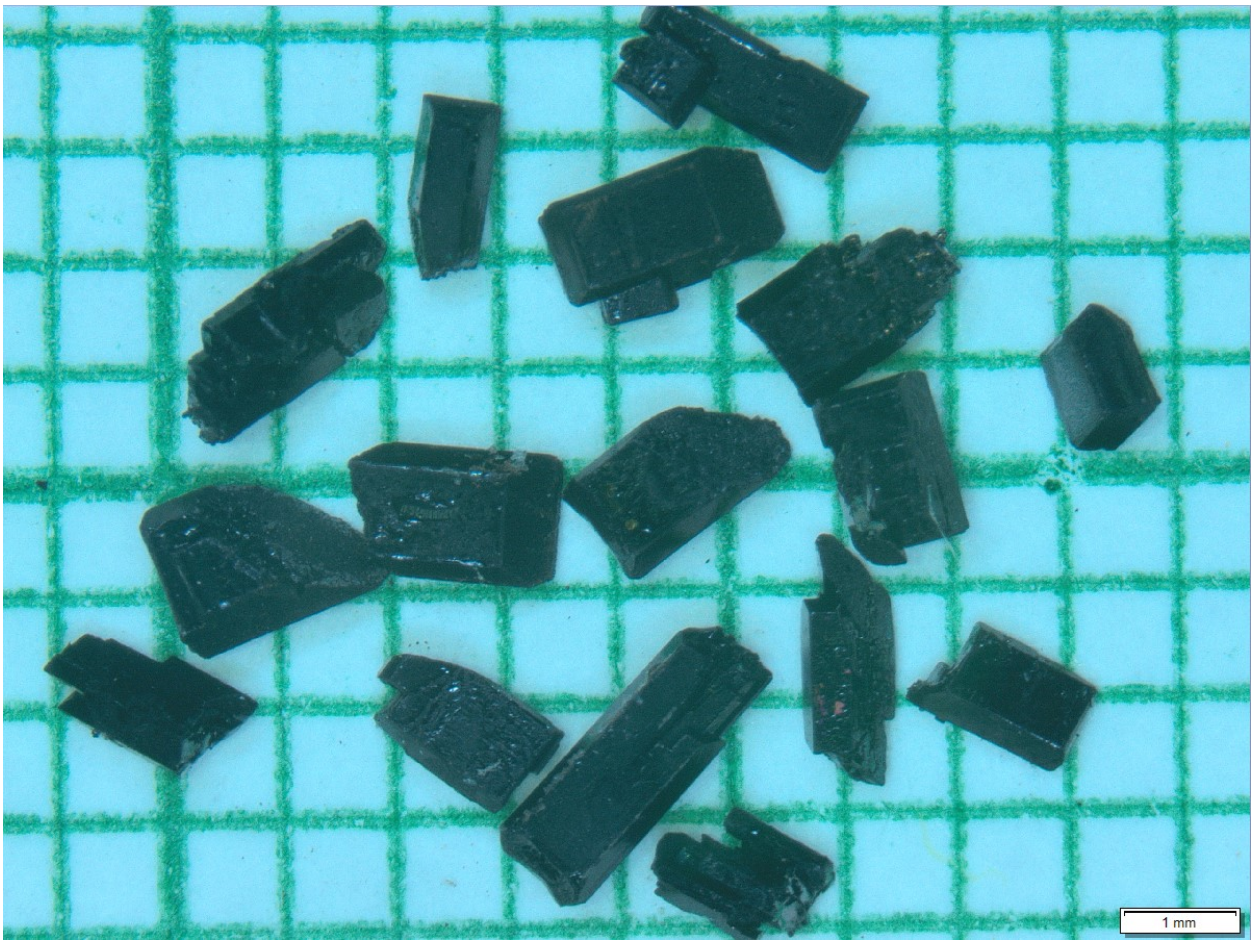

Figure S7. Typical size of single crystals $Y_4Fe_xGe_8$ ($1.0 \leq x \leq 1.5$) synthesized with the metal flux method.

Table S1. Single crystal diffraction data of $Y_4Fe_{1.44}Ge_8$ in the space group *Cmcm* (column 2 in Table 1) collected using a laboratory single crystal x-ray diffractometer.

Empirical formula	$Fe_{1.44}Ge_8Y_4$
Formula weight	1016.78
Temperature/K	296.15
Crystal system	orthorhombic
Space group	Cmcm
a/Å	4.1384(2)
b/Å	15.8468(8)
c/Å	4.0178(2)
Volume/Å^3	263.49(2)
Z	1
ρ_{calc}g/cm^3	6.408
μ/mm^{-1}	46.023
F(000)	449.0
Radiation	MoKα (λ = 0.71073 Å)
2Θ range for data collection/°	5.142 to 60.956
Index ranges	$-5 \leq h \leq 5$, $-22 \leq k \leq 22$, $-5 \leq l \leq 5$
Reflections collected	4690
Independent reflections	255 [R_{int} = 0.0298, R_{sigma} = 0.0101]
Data/restraints/parameters	255/0/19
Goodness-of-fit on F^2	1.135
Final R indexes [I>=2σ (I)]	R_1 = 0.0138, wR_2 = 0.0293
Final R indexes [all data]	R_1 = 0.0150, wR_2 = 0.0298
Largest diff. peak/hole / e Å^{-3}	0.96/-0.76

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0319P)^2+ 0.46P]$ where $P=(Fo^2+2Fc^2)/3$

Table S1 extended. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic

Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Y001	5000	3972.8(2)	7500	7.91(12)
Ge00	0	4476.6(3)	2500	10.81(13)
Ge1	0	2517.5(3)	-2500	27.37(16)
Fe04	0	3030.8(10)	2500	13.0(5)

Table S1 extended. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y001	7.11(18)	7.33(18)	9.30(19)	0	0	0
Ge00	6.6(2)	19.0(2)	6.8(2)	0	0	0
Ge1	25.9(3)	17.3(3)	39.0(3)	0	0	0
Fe04	14.8(8)	7.3(8)	16.7(9)	0	0	0

Table S1 extended. Bond Lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Y001	Ge00	2.99243(19)	Ge00	Ge00[2]	2.6052(6)
Y001	Ge00[1]	3.2123(4)	Ge00	Ge00[8]	2.6052(6)
Y001	Ge00[2]	3.2123(4)	Ge00	Fe04	2.2911(15)
Y001	Ge00[3]	2.99244(19)	Ge1	Ge1[9]	2.88450(10)
Y001	Ge00[4]	2.99244(19)	Ge1	Ge1[10]	2.88450(10)
Y001	Ge00[5]	2.99244(18)	Ge1	Ge1[11]	2.88450(10)
Y001	Ge1[6]	3.1005(5)	Ge1	Ge1[6]	2.88450(10)
Y001	Ge1[3]	3.0984(5)	Ge1	Fe04[12]	2.1673(6)
Y001	Ge1[4]	3.0984(5)	Ge1	Fe04[11]	2.2442(6)
Y001	Ge1[7]	3.1005(5)	Ge1	Fe04[6]	2.2442(6)
Y001	Fe04[7]	3.1751(16)	Ge1	Fe04	2.1673(6)
Y001	Fe04	3.2474(7)			

Table S2. Single crystal diffraction data of $Y_4Fe_{1.44}Ge_8$ in the space group *P*-1 (column 3 in Table 1) collected using a laboratory single crystal x-ray diffractometer.

Empirical formula	$Fe_{2.87}Ge_{16}Y_8$
Formula weight	2033.01
Temperature/K	296.15
Crystal system	triclinic
Space group	*P*-1
a/Å	5.7716(3)
b/Å	8.1916(4)
c/Å	11.5363(5)
α/°	79.5610(10)
β/°	88.3050(10)
γ/°	79.5490(10)
Volume/Å^3	527.49(4)
Z	1
ρ_{calc}g/cm^3	6.400
μ/mm^{-1}	45.972
F(000)	899.0
Radiation	MoKα (λ = 0.71073 Å)
2Θ range for data collection/°	3.59 to 70.32
Index ranges	$-9 \leq h \leq 9$, $-13 \leq k \leq 13$, $-18 \leq l \leq 18$
Reflections collected	23168
Independent reflections	4508 [R_{int} = 0.0532, R_{sigma} = 0.0501]
Data/restraints/parameters	4508/0/150
Goodness-of-fit on F^2	0.946
Final R indexes [I>=2σ (I)]	R_1 = 0.0307, wR_2 = 0.0749
Final R indexes [all data]	R_1 = 0.1473, wR_2 = 0.1091
Largest diff. peak/hole / e Å^{-3}	1.27/-1.40

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.0315P)^2]$ where $P=(Fo^2+2Fc^2)/3$

Table S2 extended. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Y001	-3232(3)	7940(2)	7132.0(19)	8.5(4)
Y002	-3237(3)	7943(2)	2129.5(19)	8.2(4)
Y003	8236(3)	2055(2)	366.3(17)	8.5(4)
Ge00	13487(4)	1045(3)	493(2)	10.9(5)
Y005	1762(3)	7951(2)	4631.2(17)	8.1(4)
Ge1	8480(3)	1054(3)	2993.9(19)	11.4(5)
Ge2	1501(3)	8956(3)	2005.9(19)	10.6(5)
Ge3	-3488(4)	8959(3)	4505(2)	11.4(5)
Ge4	-25(5)	5033(3)	3746(2)	28.4(7)
Ge5	10007(5)	4966(3)	1254(3)	28.4(7)
Ge6	5016(5)	5031(3)	1246(3)	27.5(6)
Ge7	5021(5)	4952(3)	3755(3)	26.9(6)
Fe0D	-2753(13)	6059(9)	4875(8)	7(2)
Fe0E	7772(15)	3931(10)	2627(8)	24(3)
Fe0F	2218(12)	6080(8)	2364(8)	14(2)
Fe0G	12747(15)	3956(10)	141(7)	12(2)

Table S2 extended. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y001	8.1(9)	8.1(8)	8.8(10)	-2.3(7)	-2.9(7)	0.9(7)
Y002	9.1(9)	6.3(8)	9.2(10)	-0.6(7)	-0.1(8)	-1.7(7)
Y003	7.3(10)	8.4(8)	9.9(11)	-2.4(8)	-1.8(8)	-0.4(7)
Ge00	7.8(10)	19.1(11)	6.6(11)	-3.1(9)	0.3(9)	-3.7(8)
Y005	9.0(10)	7.8(8)	7.8(11)	-1.4(8)	-0.6(8)	-2.0(7)
Ge1	6.1(10)	22.7(11)	6.1(12)	-4.8(9)	1.1(9)	-2.8(9)
Ge2	6.8(10)	17.2(10)	7.9(12)	-2.6(9)	-0.3(9)	-1.9(8)
Ge3	6.9(10)	19.1(11)	9.2(12)	-4.4(9)	-0.7(9)	-2.7(8)
Ge4	36.2(17)	17.0(12)	31.2(17)	-2.6(12)	-7.2(14)	-3.3(11)
Ge5	33.6(16)	18.4(12)	33.6(18)	-5.7(12)	-8.9(13)	-3.3(11)
Ge6	33.1(15)	16.7(11)	31.8(17)	-3.2(11)	-6.1(13)	-2.3(10)
Ge7	30.6(15)	17.5(11)	30.4(16)	-2.3(11)	-6.3(12)	0.4(10)
Fe0D	5(4)	-1(3)	15(5)	-1(3)	-2(3)	0(3)
Fe0E	29(5)	27(4)	15(5)	2(3)	-5(4)	-11(4)
Fe0F	7(4)	9(3)	28(5)	-10(3)	-1(3)	4(3)
Fe0G	19(5)	9(4)	8(5)	0(3)	1(3)	-2(3)

Table S2 extended. Bond Lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Y001	Ge00[1]	2.996(3)	Y005	Ge3[3]	3.206(3)
Y001	Ge1[2]	2.992(3)	Y005	Ge3	2.993(3)
Y001	Ge1[1]	2.996(3)	Y005	Ge3[13]	2.995(3)
Y001	Ge2[3]	3.217(3)	Y005	Ge4	3.108(3)
Y001	Ge3[4]	3.214(3)	Y005	Ge4[2]	3.100(3)
Y001	Ge3	2.995(3)	Y005	Ge7	3.116(3)
Y001	Ge4[2]	3.100(3)	Y005	Ge7[1]	3.093(3)
Y001	Ge5[1]	3.097(3)	Y005	Fe0D[2]	3.178(7)
Y001	Ge6[2]	3.103(3)	Y005	Fe0F	3.244(8)
Y001	Ge7[2]	3.090(3)	Ge1	Ge2[10]	2.607(2)
Y001	Fe0D	3.238(9)	Ge1	Ge3[10]	2.604(3)
Y001	Fe0F[2]	3.186(7)	Ge1	Fe0E	2.280(8)
Y002	Ge00[5]	2.989(3)	Ge2	Fe0F	2.280(7)
Y002	Ge00[6]	3.213(3)	Ge3	Ge3[4]	2.601(4)
Y002	Ge1[7]	3.219(3)	Ge3	Fe0D	2.298(7)
Y002	Ge2[8]	3.000(3)	Ge4	Ge4[2]	2.886(6)
Y002	Ge2	2.991(3)	Ge4	Ge5[8]	2.884(3)
Y002	Ge3	2.997(3)	Ge4	Ge7[8]	2.872(3)
Y002	Ge4	3.096(3)	Ge4	Ge7	2.901(3)
Y002	Ge5[8]	3.098(3)	Ge4	Fe0D	2.163(8)
Y002	Ge6[8]	3.092(3)	Ge4	Fe0D[2]	2.241(9)
Y002	Ge7[8]	3.106(3)	Ge4	Fe0E[8]	2.243(9)
Y002	Fe0E[8]	3.180(8)	Ge4	Fe0F	2.176(8)
Y002	Fe0F	3.236(7)	Ge5	Ge5[11]	2.884(6)
Y003	Ge00[8]	2.996(3)	Ge5	Ge6[13]	2.901(3)
Y003	Ge00	2.994(3)	Ge5	Ge6	2.871(3)
Y003	Ge00[9]	3.210(3)	Ge5	Fe0E	2.163(9)
Y003	Ge1	2.994(3)	Ge5	Fe0F[13]	2.246(9)
Y003	Ge2[5]	2.992(3)	Ge5	Fe0G[11]	2.241(9)
Y003	Ge2[10]	3.210(3)	Ge5	Fe0G	2.150(9)
Y003	Ge5	3.100(3)	Ge6	Ge6[5]	2.884(6)
Y003	Ge5[11]	3.100(3)	Ge6	Ge7	2.883(3)
Y003	Ge6[5]	3.107(3)	Ge6	Fe0E	2.234(9)
Y003	Ge6	3.093(3)	Ge6	Fe0F	2.188(8)
Y003	Fe0F[5]	3.238(9)	Ge6	Fe0G[11]	2.168(8)
Y003	Fe0G[11]	3.162(8)	Ge6	Fe0G[8]	2.245(10)
Ge00	Ge00[12]	2.603(4)	Ge7	Ge7[1]	2.888(6)
Ge00	Ge2[10]	2.607(3)	Ge7	Fe0D[13]	2.256(9)

Ge00	Fe0G	2.308(8)	Ge7	$Fe0D^{2}$	2.167(8)
Y005	$Ge1^{7}$	3.216(3)	Ge7	Fe0E	2.168(9)
Y005	$Ge1^{1}$	2.989(3)	Ge7	Fe0F	2.262(8)
Y005	Ge2	2.992(3)			

Table S3. Single crystal diffraction data of $Y_4Fe_xGe_8$ in the space group *P*-1 collected using synchrotron X-rays at 15-IDD (NSF's ChemMatCARS at the Advanced Photon Source).

Empirical formula	$FeGe_{7.27}Y_{4.12}$
Formula weight	950.84
Temperature/K	273.15
Crystal system	triclinic
Space group	P-1
a/Å	11.4441(3)
b/Å	32.7356(7)
c/Å	11.4456(3)
α/°	79.6330(10)
β/°	88.3300(10)
γ/°	79.6350(10)
Volume/Å^3	4149.01(18)
Z	16
ρ_{calc}g/cm^3	6.089
μ/mm^{-1}	44.801
F(000)	6716.0
Radiation	Synchrotron X-rays (λ = 0.41328 Å)
2Θ range for data collection/°	2.57 to 72.638
Index ranges	$-19 \leq h \leq 19$, $-54 \leq k \leq 54$, $-18 \leq l \leq 19$
Reflections collected	211855
Independent reflections	38527 [R_{int} = 0.0667, R_{sigma} = 0.0640]
Data/restraints/parameters	38527/0/1258
Goodness-of-fit on F^2	0.900
Final R indexes [I>=2σ (I)]	R_1 = 0.0844, wR_2 = 0.3076
Final R indexes [all data]	R_1 = 0.3148, wR_2 = 0.5523
Largest diff. peak/hole / e Å^{-3}	16.01/-2.72

Table S3 extended. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**

Table S3 extended. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Y001	9114(2)	9260.8(9)	5371(2)	0.8(5)
Y002	6613(2)	1776.4(9)	12865(3)	-0.2(5)
Y003	4120(2)	1759.9(8)	10363(3)	-0.6(5)
Y004	9111(2)	6772.8(9)	5370(2)	-0.4(5)
Y005	10892(2)	5725.7(9)	-363(3)	-1.0(5)
Y006	10891(3)	5726.0(9)	4638(3)	0.1(5)
Y007	10881(2)	8241.3(8)	-369(3)	-0.3(5)
Y008	5883(2)	3230.0(9)	-362(2)	-0.9(5)
Y009	5883(2)	3225.8(9)	4633(2)	-0.7(5)
Y00A	6625(2)	4259.3(9)	2871(2)	-0.8(5)
Y00B	8390(2)	-1772.6(9)	12134(2)	-0.9(5)
Y00C	3386(2)	726.2(9)	12140(3)	-0.3(5)
Y00D	4117(2)	1758.2(8)	5377(3)	-0.5(5)
Y00E	8392(2)	725.6(8)	12138(2)	-0.5(5)
Y00F	6624(2)	6760.5(8)	-2129(3)	-0.3(5)
Y00G	5879(2)	741.0(9)	4629(2)	-0.3(5)
Y00H	9120(2)	9261.5(9)	366(2)	-0.7(5)
Y00I	6613(2)	-725.5(9)	12860(2)	-0.6(5)
Y00J	6617(2)	6761.8(8)	2865(3)	-0.2(5)
Y00K	1605(3)	-725.7(8)	12866(2)	-0.2(5)
Y00L	6626(2)	4259.3(9)	7867(2)	-0.8(5)
Y00M	4112(3)	4276.0(9)	361(3)	-0.5(5)
Y00N	9113(2)	6773.7(9)	362(2)	0.2(5)
Y00O	8380(2)	3238.3(8)	2129(3)	-1.0(5)
Y00P	8381(2)	5740.8(9)	-2869(2)	-0.6(5)
Y00Q	3386(2)	-1774.4(9)	12134(2)	-0.6(5)
Y00R	8379(2)	3236.9(8)	7136(3)	-0.3(5)
Y00S	4109(2)	4275.0(9)	5363(3)	-0.8(5)
Y00T	10881(2)	-1760.3(8)	14629(3)	-1.0(5)
Y00U	5883(2)	740.3(9)	9635(2)	0.1(5)
Y00V	8380(2)	5741.4(9)	2131(2)	-0.9(5)
Y00W	1610(2)	1774.3(9)	12867(2)	-0.5(5)
Ge0X	-761(3)	1513.2(11)	13003(3)	2.9(8)
Ge0Y	4239(3)	1512.1(11)	12999(3)	1.0(8)
Ge0Z	8253(3)	988.6(11)	4505(3)	0.6(8)
Ge10	10762(3)	-1510.8(11)	11998(3)	1.3(8)
Ge11	10756(3)	5987.4(13)	2004(3)	2.3(9)
Ge12	4237(3)	4013.8(12)	8002(3)	0.9(8)
Ge13	4237(3)	-991.1(12)	12993(3)	3.5(9)
Ge14	6744(3)	9013.1(12)	500(3)	2.9(9)
Ge15	10761(3)	5991.0(12)	-3006(3)	3.0(8)

Table S3 extended. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ge16	8258(3)	8490.4(12)	-504(3)	3.7(9)
Ge17	6743(3)	6511.7(11)	5503(3)	1.5(8)
Ge18	9247(3)	-991.3(12)	12990(3)	3.9(9)
Ge19	8263(3)	5988.2(12)	-495(3)	5.1(9)
Ge1A	8265(3)	5990.8(12)	4494(3)	4.4(9)
Ge1B	5753(3)	3490.2(13)	7000(3)	3.0(9)
Ge1C	9246(3)	6506.8(13)	-1990(3)	2.1(8)
Ge1D	6749(3)	6509.9(11)	503(3)	1.4(8)
Ge1E	756(3)	993.0(12)	11997(3)	2.8(8)
Ge1F	6745(3)	1508.9(13)	10505(3)	3.1(9)
Ge1G	5758(3)	-1508.5(11)	11996(4)	2.5(8)
Ge1H	6737(3)	9012.1(12)	5503(3)	1.9(8)
Ge1I	8258(3)	989.0(12)	9498(3)	1.9(8)
Ge1J	9245(3)	6510.0(12)	3000(3)	3.4(9)
Ge1K	6744(3)	1509.2(12)	5501(3)	2.8(8)
Ge1L	5761(3)	991.0(12)	11993(3)	5.3(9)
Ge1M	8255(3)	8493.4(13)	4491(3)	3.8(9)
Ge1N	6743(3)	4005.9(12)	5504(3)	3.3(9)
Ge1O	4238(3)	4016.5(12)	3000(3)	3.4(9)
Ge1P	8259(3)	3490.7(11)	-498(3)	2.6(8)
Ge1Q	8262(3)	3484.7(11)	4507(3)	1.9(8)
Y01R	5748(3)	3496.9(12)	2000(3)	9.5(7)
Ge1S	6743(3)	4008.7(12)	499(3)	3.9(9)
Ge1T	7391(3)	7511.4(15)	-3744(4)	12.5(11)
Ge1U	5011(4)	-11.9(13)	11172(5)	20.2(13)
Ge1V	4982(4)	4990.2(14)	1372(3)	11.1(10)
Ge1W	4890(20)	2464(12)	11290(30)	21(7)
Ge1X	7612(4)	2486.3(15)	3756(4)	14.0(12)
Ge1Y	7504(5)	12.5(14)	11158(4)	21.1(11)
Ge1Z	7600(4)	2509.2(14)	1202(5)	19.2(12)
Ge20	7472(5)	5015.3(13)	1342(4)	15.3(12)
Ge21	10014(5)	5009.6(14)	3673(4)	20.1(13)
Ge22	4991(4)	13.4(12)	13836(5)	16.6(11)
Ge23	7488(4)	5015.2(12)	6330(3)	10.0(9)
Ge24	7572(5)	2513.8(14)	6224(5)	16.4(12)
Ge25	4927(4)	2490.6(13)	6246(5)	17.0(12)
Ge26	10078(4)	7511.6(13)	-1260(4)	16.1(11)
Ge28	10114(4)	7489.1(14)	6225(4)	14.7(11)
Ge29	10071(4)	7487.5(14)	1235(4)	14.6(12)
Ge2A	7530(4)	4990.9(12)	3638(4)	15.1(11)
Ge2B	2485(5)	-12.5(14)	13846(4)	17.7(14)

Table S3 extended. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ge2C	7478(5)	-8.9(14)	13859(4)	19.1(13)
Ge2D	2517(5)	10.8(14)	11148(4)	15.5(13)
Ge2E	7422(5)	7487.9(14)	3764(5)	17.9(13)
Ge2F	22(5)	-12.0(13)	11164(4)	15.7(12)
Ge2G	5023(4)	5012.0(13)	3626(3)	13.2(11)
Ge2H	10004(4)	5011.0(14)	-1329(4)	14.5(11)
Ge2I	4780(40)	2508(6)	8950(40)	9(4)
Ge2J	7531(5)	4987.1(13)	-1340(4)	19.1(13)
Ge2L	9968(4)	13.2(13)	13839(4)	13.9(11)
Ge2M	7566(5)	2487.4(15)	8756(5)	23.5(15)
Ge2N	10079(4)	7509.2(13)	3733(5)	16.9(12)
Ge2O	7428(5)	7512.8(15)	1248(5)	23.0(14)
Fe2P	6122(8)	2760(3)	2380(8)	5(2)
Fe2Q	6115(10)	265(3)	12365(10)	5(3)
Fe2R	8888(8)	7235(3)	-2370(8)	6(2)
Fe2S	6382(8)	4740(3)	5133(8)	4(2)
Fe2T	6396(8)	4741(3)	124(8)	6(2)
Fe2U	8601(9)	5268(3)	-121(9)	2(2)
Fe2V	6130(9)	2763(4)	7368(9)	1(3)
Fe2W	8890(9)	7235(3)	2613(10)	3(3)
Fe2X	6392(10)	2236(4)	10146(10)	0(3)
Fe2Y	8611(10)	5265(4)	4871(10)	5(3)
Fe2Z	1116(9)	259(3)	12375(9)	5(2)
Fe30	6381(9)	2240(3)	5122(10)	4(3)
Fe31	8904(10)	-265(3)	12630(9)	3(2)
Fe32	8619(9)	7762(3)	4878(9)	2(3)
Fe33	3883(10)	-267(3)	12615(10)	2(3)
Fe34	8591(11)	7756(4)	-135(10)	7(3)
Fe1	8850(20)	2231(8)	7640(20)	12(6)
Fe2	6120(20)	7778(7)	2380(20)	5(5)
Fe3	3500(50)	2790(20)	4950(40)	50(30)
Fe9	11430(40)	7233(12)	220(50)	28(13)
Fe12	3850(50)	2211(16)	12680(50)	20(14)
Fe13	8880(40)	4720(14)	2660(30)	21(13)
Fe14	8930(20)	4708(12)	-2350(20)	28(10)
Fe6	6420(30)	7232(11)	100(30)	8(8)
Fe15	6160(40)	5279(16)	2460(50)	-1(12)
Ge1	4880(3)	2513.3(13)	3785(4)	12.8(11)
Ge2	7410(5)	7489.7(14)	-1218(5)	15.9(12)
Ge7	5020(20)	2514(5)	8690(20)	6(2)
Ge8	4953(13)	2500(5)	11226(15)	24(4)

Table S3 extended. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe19	8550(40)	278(15)	14860(40)	4(11)
Fe7	6490(40)	-320(15)	10190(50)	19(15)
Fe4	6520(40)	-255(16)	15090(40)	0(12)
Fe10	11450(70)	7779(12)	-2750(40)	90(30)
Fe8	11580(160)	7200(20)	4990(60)	200(80)
Fe11	1630(80)	-292(18)	10090(50)	50(30)

Table 3 extended. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y001	0.7(10)	1.4(11)	0.4(11)	0.5(10)	0.6(8)	-1.5(9)
Y002	-0.3(10)	-0.8(11)	0.6(11)	-0.4(9)	1.0(8)	-0.2(9)
Y003	-0.3(10)	-0.3(11)	-1.0(10)	0.3(10)	-0.1(8)	-0.5(9)
Y004	-0.6(10)	0.7(11)	-0.7(11)	-0.5(9)	0.3(8)	-0.6(9)
Y005	-1.0(9)	-0.9(11)	-1.0(10)	0.2(9)	0.0(7)	0.1(9)
Y006	-0.9(9)	2.2(11)	-0.9(10)	-0.5(10)	0.1(7)	-0.3(9)
Y007	0.3(10)	-0.4(10)	-0.5(10)	-0.3(10)	0.8(8)	-0.7(9)
Y008	-1.0(10)	-1.0(11)	-0.8(11)	0.2(9)	0.0(8)	0.2(9)
Y009	-1.0(10)	-0.5(12)	-0.9(11)	0.4(9)	0.0(8)	0.2(9)
Y00A	-0.8(10)	-1.0(11)	-0.7(11)	0.1(10)	0.3(8)	0.1(9)
Y00B	-1.0(10)	-0.6(11)	-0.9(11)	0.0(9)	0.0(8)	0.1(9)
Y00C	-0.9(10)	-0.4(11)	-0.2(11)	0.9(10)	0.3(8)	0.4(9)
Y00D	-0.3(10)	-0.8(11)	-0.1(10)	-0.3(10)	0.8(8)	-0.3(9)
Y00E	-0.5(10)	0.1(11)	-0.9(10)	-0.1(10)	0.2(8)	-0.6(9)
Y00F	-0.1(10)	0.2(11)	-0.5(10)	-0.3(10)	0.6(8)	-0.7(9)
Y00G	-0.2(10)	0.1(11)	-0.7(10)	0.5(9)	0.2(8)	-0.3(9)
Y00H	-1.0(10)	-0.4(11)	-0.8(10)	0.3(9)	0.1(8)	0.2(9)
Y00I	-1.0(10)	0.1(11)	-1.0(10)	0.3(10)	0.0(8)	-0.1(9)
Y00J	-1.0(10)	1.1(11)	-0.9(10)	0.6(10)	0.0(8)	-0.1(9)
Y00K	-0.2(10)	-0.6(11)	0.1(10)	0.8(10)	-0.5(8)	-0.3(9)
Y00L	-0.6(10)	-1.0(11)	-0.7(11)	0.2(10)	0.3(8)	0.2(9)
Y00M	-0.5(9)	0.3(11)	-1.0(10)	0.1(10)	0.1(7)	-0.6(10)
Y00N	-0.3(10)	2.2(11)	-0.9(11)	-0.3(10)	0.2(8)	-1.4(9)
Y00O	-1.0(10)	-0.9(10)	-1.0(10)	0.2(10)	0.0(8)	0.2(9)
Y00P	-1.0(10)	0.0(11)	-0.5(11)	-0.6(10)	0.1(8)	0.0(9)
Y00Q	-1.0(10)	-0.5(11)	-0.5(11)	0.7(9)	0.1(8)	0.3(9)
Y00R	-0.4(10)	-1.0(10)	0.6(10)	0.0(10)	1.0(8)	0.1(9)
Y00S	-0.8(9)	-0.5(11)	-0.9(10)	0.0(10)	0.1(7)	-0.1(9)
Y00T	-1.0(10)	-1.0(10)	-1.0(10)	0.2(10)	0.0(8)	0.2(9)
Y00U	-0.3(10)	-0.2(11)	0.5(11)	1.3(10)	-1.0(8)	-0.6(9)
Y00V	-1.0(10)	-0.8(11)	-0.9(11)	0.3(10)	0.0(8)	0.1(9)
Y00W	-1.0(10)	0.5(11)	-1.0(11)	0.1(9)	0.0(8)	0.1(9)
Ge0X	1.6(14)	6.0(16)	1.1(13)	0.5(14)	1.8(10)	-2.2(13)
Ge0Y	-0.9(13)	3.9(16)	-0.9(13)	0.9(13)	0.1(9)	0.7(12)
Ge0Z	-0.3(13)	2.6(17)	-0.4(14)	-0.7(12)	-0.5(10)	0.1(12)
Ge10	0.2(13)	4.8(15)	-0.8(13)	-0.9(13)	0.1(9)	-0.8(12)
Ge11	0.5(14)	7.2(19)	-0.2(15)	-0.2(13)	0.8(10)	-2.5(12)
Ge12	-0.3(14)	3.6(17)	-0.4(14)	-0.4(13)	0.6(10)	-1.0(12)
Ge13	0.4(14)	8.4(18)	2.0(15)	-1.6(14)	1.0(10)	-1.2(13)

Table 3 extended. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ge14	1.2(15)	5.8(18)	2.7(16)	-0.6(13)	0.1(11)	-3.7(13)
Ge15	0.5(13)	9.6(17)	-0.4(14)	-1.2(13)	1.0(10)	-2.3(12)
Ge16	3.2(14)	6.6(17)	1.7(15)	-0.3(13)	-0.8(10)	-2.6(13)
Ge17	-0.3(14)	4.7(16)	-0.3(14)	0.0(14)	0.7(10)	0.3(13)
Ge18	0.3(14)	10.4(19)	1.6(15)	-2.7(14)	-0.4(10)	-0.4(14)
Ge19	1.8(14)	12.7(18)	1.3(14)	0.0(14)	0.1(10)	-4.1(13)
Ge1A	0.6(13)	12.9(18)	1.2(14)	-4.9(14)	1.4(10)	-1.6(13)
Ge1B	0.8(14)	9.7(19)	-0.5(15)	-2.1(14)	0.5(11)	-2.3(13)
Ge1C	-0.7(14)	8.3(18)	-0.5(15)	-1.8(13)	0.4(10)	-1.2(13)
Ge1D	1.3(13)	4.9(15)	-1.0(13)	0.0(13)	0.1(10)	-3.5(12)
Ge1E	-0.4(13)	9.9(18)	-0.2(14)	-2.2(14)	0.7(10)	-1.9(13)
Ge1F	-0.5(14)	8.6(18)	1.6(16)	-1.4(14)	1.0(11)	-1.6(13)
Ge1G	0.3(14)	7.7(17)	-0.5(14)	0.8(14)	0.2(10)	-1.9(13)
Ge1H	1.4(14)	5.3(17)	0.2(14)	-1.2(13)	1.5(10)	-3.2(12)
Ge1I	0.9(14)	3.6(17)	1.5(15)	-0.7(13)	2.0(10)	-1.4(12)
Ge1J	-0.2(14)	9.2(18)	1.5(15)	-1.7(14)	1.4(10)	-0.9(13)
Ge1K	-0.5(13)	8.0(17)	1.0(15)	-0.4(13)	0.6(10)	-1.7(12)
Ge1L	2.6(14)	13.2(19)	0.9(15)	0.0(14)	2.0(10)	-4.6(14)
Ge1M	2.6(14)	9.1(18)	-0.2(15)	-1.0(14)	1.7(10)	-1.5(13)
Ge1N	0.3(14)	9.7(18)	-0.1(15)	0.5(14)	0.8(10)	-2.0(13)
Ge1O	0.4(14)	8.1(17)	1.1(14)	1.2(12)	1.3(10)	-1.5(12)
Ge1P	0.8(14)	6.3(16)	0.7(14)	-0.3(13)	1.5(10)	-1.3(13)
Ge1Q	0.6(13)	5.5(15)	0.1(13)	-1.0(13)	1.2(9)	-1.3(12)
Y01R	2.2(12)	20.4(18)	6.4(13)	-2.8(13)	3.9(10)	-3.3(12)
Ge1S	1.4(14)	10.5(18)	0.8(14)	-1.2(14)	1.8(10)	-3.6(13)
Ge1T	2.3(17)	9(2)	27(2)	-4.1(18)	-0.7(15)	-2.6(14)
Ge1U	24(2)	6.5(18)	28(3)	-3.4(17)	-4.8(18)	4.8(17)
Ge1V	20(2)	12(2)	2.1(15)	0.8(14)	6.5(13)	-8.0(16)
Ge1W	8(9)	26(14)	29(11)	2(9)	13(12)	-9(8)
Ge1X	3.4(18)	9(2)	31(3)	-4.7(18)	0.5(16)	-1.8(15)
Ge1Y	42(3)	10(2)	12(2)	-3.6(16)	-1.2(18)	-3.9(18)
Ge1Z	16.8(19)	8.1(19)	30(2)	3.1(18)	-2.2(15)	-2.5(15)
Ge20	30(3)	6.1(18)	7.0(17)	-1.2(15)	-1.5(15)	5.4(17)
Ge21	33(3)	7.3(18)	20(2)	-2.4(16)	-9.9(19)	-1.7(18)
Ge22	26(2)	4.2(17)	18(2)	-3.7(15)	-5.0(16)	5.6(15)
Ge23	10.3(17)	11.7(18)	5.6(15)	0.0(14)	8.2(12)	1.5(14)
Ge24	18(2)	3.2(18)	26(2)	1.2(17)	-4.0(16)	1.1(16)
Ge25	12.7(18)	6.3(18)	30(3)	0.5(18)	-6.5(16)	1.4(15)
Ge26	2.2(14)	10.9(19)	33(3)	1.3(18)	6.5(13)	-2.6(14)

Table 3 extended. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ge28	3.3(16)	9.0(19)	32(2)	-8.1(18)	3.8(14)	1.5(14)
Ge29	12.8(19)	4.1(19)	26(2)	-3.5(17)	-2.4(15)	2.1(15)
Ge2A	24(2)	6.6(17)	12.8(18)	-2.2(15)	-3.7(15)	4.7(15)
Ge2B	33(3)	5.5(19)	15(2)	-4.1(16)	-6(2)	-1.4(18)
Ge2C	36(3)	5.6(19)	16(2)	0.6(16)	-5.9(19)	-5.2(18)
Ge2D	29(3)	1.6(19)	16(3)	0.4(16)	-1.7(19)	-3.0(17)
Ge2E	16(2)	5.9(19)	30(3)	3.3(19)	0.2(17)	-3.8(17)
Ge2F	24(3)	6.7(19)	14(2)	-3.8(16)	-4.9(18)	4.6(17)
Ge2G	32(3)	8.5(18)	0.3(15)	-1.5(13)	6.4(14)	-7.4(17)
Ge2H	19(2)	6.7(19)	20(2)	-5.2(16)	0.4(15)	-5.4(15)
Ge2I	14(7)	-1(4)	13(8)	0(4)	15(6)	0(4)
Ge2J	38(3)	3.1(18)	14.4(19)	-2.2(16)	-11.3(17)	3.2(19)
Ge2L	19(2)	6.7(18)	13(2)	-3.4(15)	0.9(16)	5.4(15)
Ge2M	34(3)	2.4(19)	34(3)	-8.0(19)	-13(2)	5.0(18)
Ge2N	11.7(18)	5.0(19)	32(3)	1.6(18)	-13.7(16)	1.7(15)
Ge2O	39(3)	1.7(19)	29(3)	-4.5(18)	-8(2)	-1.9(18)
Fe2P	4(3)	13(5)	0(4)	-3(3)	2(3)	-5(3)
Fe2Q	8(4)	4(5)	3(5)	1(4)	-4(3)	-6(4)
Fe2R	5(4)	7(4)	5(4)	1(3)	6(3)	-1(3)
Fe2S	2(3)	9(4)	1(4)	-2(3)	3(3)	-1(3)
Fe2T	3(3)	11(4)	3(4)	-1(3)	4(2)	0(3)
Fe2U	1(4)	4(4)	2(4)	2(3)	-2(3)	-2(3)
Fe2V	4(4)	-1(5)	1(5)	1(4)	-3(3)	-1(3)
Fe2W	1(4)	0(5)	7(5)	0(4)	-1(3)	1(3)
Fe2X	-1(5)	0(5)	0(5)	1(4)	1(4)	1(4)
Fe2Y	1(4)	10(6)	4(5)	3(4)	-3(3)	-1(4)
Fe2Z	1(4)	9(5)	3(4)	1(3)	3(3)	0(3)
Fe30	0(4)	2(4)	9(5)	1(4)	-2(3)	-2(3)
Fe31	10(4)	0(4)	-1(4)	0(3)	1(3)	-3(4)
Fe32	-1(4)	3(5)	3(5)	4(4)	1(3)	1(3)
Fe33	2(4)	-1(5)	5(5)	-1(4)	5(3)	-1(3)
Fe34	13(5)	5(6)	0(5)	1(4)	3(4)	7(4)
Fe1	5(9)	15(13)	10(9)	9(9)	8(6)	3(9)
Fe2	-1(8)	3(9)	11(10)	-1(8)	2(7)	0(7)
Fe3	20(30)	90(60)	10(20)	10(20)	5(16)	50(30)
Fe9	17(17)	3(16)	60(30)	16(18)	-34(17)	-8(13)
Fe12	30(30)	0(20)	20(20)	4(18)	20(17)	10(20)
Fe13	40(30)	20(20)	0(16)	3(15)	-2(14)	4(18)
Fe14	0(10)	80(30)	-1(11)	2(12)	0(8)	-7(11)

Table 3 extended. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe6	-1(13)	17(16)	6(14)	5(12)	0(10)	-1(11)
Fe15	0(20)	0(20)	0(20)	0(17)	0(16)	0(15)
Ge1	4.5(16)	6.0(18)	28(2)	-5.8(16)	-1.5(14)	0.3(14)
Ge2	12(2)	6.5(19)	26(2)	1.6(18)	-4.9(15)	1.4(16)
Ge7	4(5)	12(4)	4(5)	-4(3)	5(4)	-3(3)
Ge8	28(7)	1(5)	41(8)	-6(4)	-29(8)	7(4)
Fe19	10(20)	0(19)	-1(19)	0(15)	-1(14)	-4(14)
Fe7	0(20)	8(19)	40(30)	5(18)	10(20)	3(15)
Fe4	-1(18)	0(20)	1(19)	2(14)	0(14)	1(14)
Fe10	240(80)	0(15)	40(20)	-5(14)	-90(40)	10(30)
Fe8	600(200)	10(30)	20(30)	10(20)	-120(60)	-70(70)
Fe11	110(80)	10(20)	40(30)	10(20)	30(40)	-10(30)

Table S4. Atomic coordinates for the √2×√2 supercell of the orthorhombic *Cmcm* structure with a formula of $Y_4Fe_{1.5}Ge_8$ used in DFT calculations.

		x	y	z	Occ.	U	Site	Sym.
1	Y Y1	0.62500	0.87500	0.39728	1.000	0.000	1a	1
2	Y Y2	0.12500	0.37500	0.39728	1.000	0.000	1a	1
3	Y Y3	0.37500	0.12500	0.60272	1.000	0.000	1a	1
4	Y Y4	0.87500	0.62500	0.60272	1.000	0.000	1a	1
5	Y Y5	0.37500	0.62500	0.89728	1.000	0.000	1a	1
6	Y Y6	0.87500	0.12500	0.89728	1.000	0.000	1a	1
7	Y Y7	0.12500	0.87500	0.10272	1.000	0.000	1a	1
8	Y Y8	0.62500	0.37500	0.10272	1.000	0.000	1a	1
9	Ge Ge1	0.12500	0.87500	0.44766	1.000	0.000	1a	1
10	Ge Ge2	0.62500	0.37500	0.44766	1.000	0.000	1a	1
11	Ge Ge3	0.37500	0.62500	0.55234	1.000	0.000	1a	1
12	Ge Ge4	0.87500	0.12500	0.55234	1.000	0.000	1a	1
13	Ge Ge5	0.37500	0.12500	0.94766	1.000	0.000	1a	1
14	Ge Ge6	0.87500	0.62500	0.94766	1.000	0.000	1a	1
15	Ge Ge7	0.62500	0.87500	0.05234	1.000	0.000	1a	1
16	Ge Ge8	0.12500	0.37500	0.05234	1.000	0.000	1a	1
17	Ge Ge9	0.37500	0.62500	0.25175	1.000	0.000	1a	1
18	Ge Ge10	0.87500	0.12500	0.25175	1.000	0.000	1a	1
19	Ge Ge11	0.12500	0.87500	0.74825	1.000	0.000	1a	1
20	Ge Ge12	0.62500	0.37500	0.74825	1.000	0.000	1a	1
21	Ge Ge13	0.62500	0.87500	0.75175	1.000	0.000	1a	1
22	Ge Ge14	0.12500	0.37500	0.75175	1.000	0.000	1a	1
23	Ge Ge15	0.37500	0.12500	0.24825	1.000	0.000	1a	1
24	Ge Ge16	0.87500	0.62500	0.24825	1.000	0.000	1a	1
25	Fe Fe1	0.12500	0.87500	0.30308	1.000	0.000	1a	1
26	Fe Fe2	0.62500	0.37500	0.30308	1.000	0.000	1a	1
27	Fe Fe3	0.37500	0.62500	0.69692	1.000	0.000	1a	1

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