Electronic Supplementary Information (ESI) available:

Flux Growth a nd Characterization of $FeSi_4P_4$ Single Crystal

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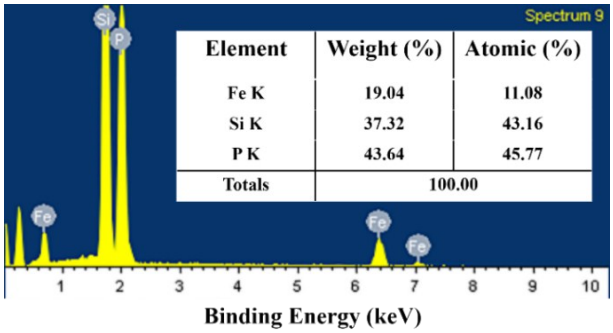

Fig. S1 The EDS spectrum of the FSP crystal. No Sn element is detected in the spectrum.

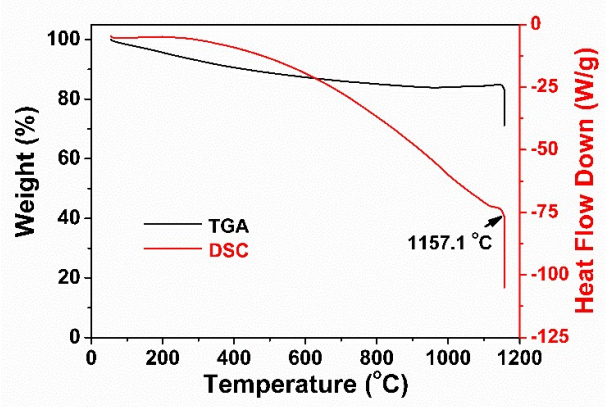

Fig. S2 DSC and TGA data for FSP single crystal. The FSP crystal decomposes at about 1157.1 ºC.

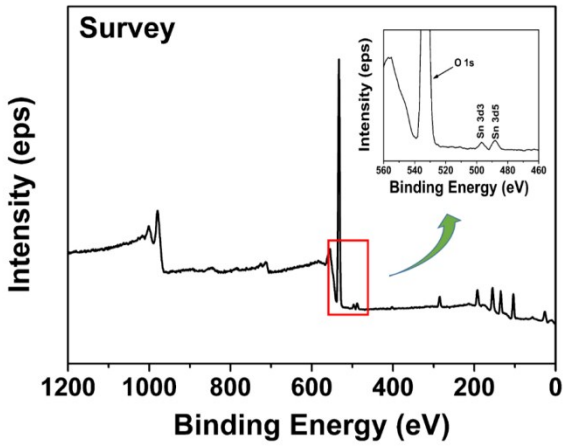

Fig. S3 The survey XPS spectrum of the $FeSi_4P_4$ crystal without being soaked in dilute hydrochloric acid. The Binding Energy of Sn 3d peaks are between 480 eV and 500 eV.

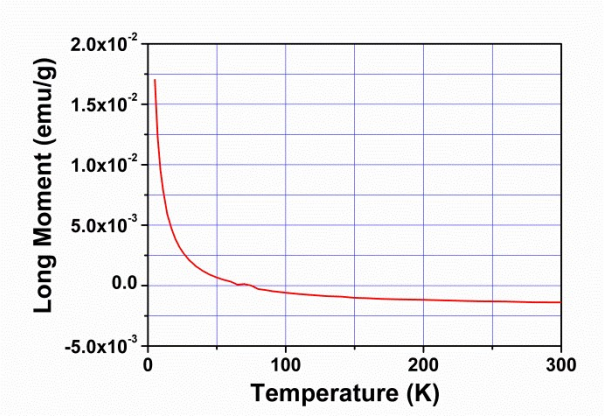

Fig. S4 The M-T curve of the $FeSi_4P_4$ crystal without being soaked in dilute hydrochloric acid. The value of the magnetization descends to 0 at about 70 K.

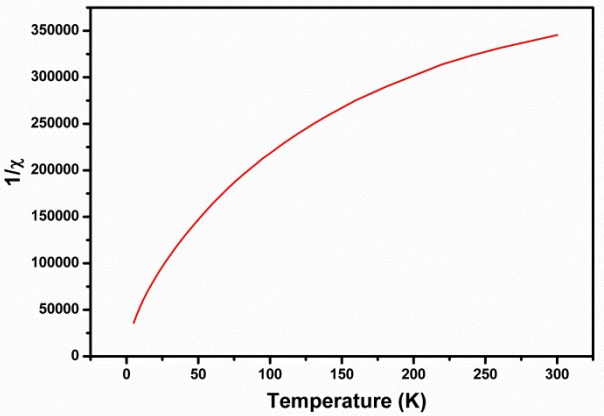

Fig. S5 The curve of temperature dependent inverse susceptibility.

Table S1 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.3202 (3)	0.4460 (2)	0.1770 (3)	0.00435 (15)
Si1	0.6668 (4)	0.0441 (3)	0.0611 (3)	0.0063 (4)
Si2	0.5591 (4)	0.7860 (3)	-0.3930 (3)	0.0064 (4)
Si3	0.1652 (4)	0.4189 (3)	-0.1267 (3)	0.0066 (4)
Si4	-0.0031 (4)	0.2240 (3)	0.3952 (3)	0.0063 (4)
P1	0.6484 (4)	0.6666 (3)	-0.0552 (3)	0.0056 (3)
P2	1.0830 (4)	0.0878 (3)	-0.2585 (3)	0.0055 (3)
P3	0.4757 (4)	0.4593 (3)	0.4869 (3)	0.0057 (3)
P4	-0.0453 (3)	0.8470 (3)	0.2934 (3)	0.0059 (3)

Table S2 Atomic displacement parameters (Å^2).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0039 (2)	0.0041 (2)	0.0039 (2)	-0.00086 (17)	-0.00051 (17)	-0.00007 (16)
Si1	0.0066 (8)	0.0055 (8)	0.0060 (8)	-0.0022 (7)	-0.0014 (7)	0.0006 (7)
Si2	0.0060 (8)	0.0037 (8)	0.0067 (9)	0.0003 (6)	-0.0011 (7)	0.0004 (7)
Si3	0.0059 (8)	0.0072 (8)	0.0069 (9)	-0.0013 (7)	-0.0031 (7)	-0.0007 (6)
Si4	0.0063 (8)	0.0082 (9)	0.0045 (8)	-0.0025 (7)	-0.0016 (7)	-0.0006 (7)
P1	0.0054 (8)	0.0028 (7)	0.0069 (8)	-0.0004 (6)	-0.0014 (6)	0.0010 (6)
P2	0.0051 (7)	0.0073 (7)	0.0037 (7)	-0.0022 (6)	-0.0009 (6)	-0.0002 (6)
P3	0.0064 (8)	0.0050 (7)	0.0035 (7)	-0.0017 (6)	0.0005 (6)	0.0003 (6)
P4	0.0059 (8)	0.0048 (7)	0.0060 (8)	-0.0004 (6)	-0.0021 (7)	-0.0004 (6)

Table S3 The bond lengths of $FeSi_4P_4$ crystal.

Fe1—Si1	2.276 (6)	Si3—P3^{iii}	2.321 (6)
Fe1—Si3	2.282 (6)	Si4—P3^{vi}	2.305 (7)
Fe1—P4	2.301 (6)	Si4—P2^{vii}	2.324 (7)
Fe1—Si4	2.302 (5)	Si4—P4^{i}	2.336 (7)
Fe1—P3	2.302 (6)	P1—Si1^{viii}	2.318 (7)
Fe1—P1	2.336 (5)	P1—Si3^{ix}	2.321 (7)
Si1—P2	2.303 (6)	P2—Si2^{ii}	2.250 (6)
Si1—P1^{i}	2.318 (7)	P2—Si3^{ix}	2.283 (6)
Si1—P4^{ii}	2.320 (5)	P2—Si4^{v}	2.324 (7)
Si2—P3^{iii}	2.231 (6)	P3—Si2^{x}	2.231 (6)
Si2—P2^{iv}	2.250 (6)	P3—Si4^{ix}	2.305 (7)
Si2—P4^{v}	2.258 (6)	P3—Si3^{x}	2.321 (6)
Si2—P1	2.265 (7)	P4—Si2^{vii}	2.258 (6)
Si3—P2^{vi}	2.283 (6)	P4—Si1^{iv}	2.320 (5)
Si3—P1^{vi}	2.321 (7)	P4—Si4^{viii}	2.336 (7)

Table S4 The bond angles of $FeSi_4P_4$ crystal.

Atoms 1,2,3	**Angle 1,2,3 [°]**	**Atoms 1,2,3**	**Angle 1,2,3 [°]**
Si1—Fe1—Si3	87.40 (16)	P1^{vi}—Si3—P3^{iii}	109.82 (14)
Si1—Fe1—P4	177.76 (11)	Fe1—Si4—P3^{vi}	112.3 (2)
Si3—Fe1—P4	91.10 (17)	Fe1—Si4—P2^{vii}	111.74 (18)

Si1—Fe1—Si4	82.0 (2)	P3^{vi}—Si4—P2^{vii}	109.29 (14)
Si3—Fe1—Si4	87.7 (2)	Fe1—Si4—P4^{i}	129.50 (17)
P4—Fe1—Si4	96.3 (3)	P3^{vi}—Si4—P4^{i}	94.9 (2)
Si1—Fe1—P3	91.20 (16)	P2^{vii}—Si4—P4^{i}	96.78 (17)
Si3—Fe1—P3	177.99 (10)	Si2—P1—Si1^{viii}	99.84 (17)
P4—Fe1—P3	90.25 (16)	Si2—P1—Si3^{ix}	112.46 (14)
Si4—Fe1—P3	90.7 (2)	Si1^{viii}—P1—Si3^{ix}	97.7 (2)
Si1—Fe1—P1	97.4 (2)	Si2—P1—Fe1	111.36 (18)
Si3—Fe1—P1	90.7 (2)	Si1^{viii}—P1—Fe1	125.24 (18)
P4—Fe1—P1	84.3 (2)	Si3^{ix}—P1—Fe1	109.4 (2)
Si4—Fe1—P1	178.23 (11)	Si2^{ii}—P2—Si3^{ix}	104.2 (2)
P3—Fe1—P1	91.0 (2)	Si2^{ii}—P2—Si1	123.94 (18)

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) *x*+1, *y*-1, *z*; (iii) *x*, *y*, *z*-1; (iv) *x*-1, *y*+1, *z*; (v) *x*+1, *y*, *z*-1; (vi) *x*-1, *y*, *z*; (vii) *x*-1, *y*, *z*+1; (viii) *x*, *y*+1, *z*; (ix) *x*+1, *y*, *z*; (x) *x*, *y*, *z*+1