Supporting Information for

Pressure-induced redox reversal of iron and the distribution of elements in deep Earth

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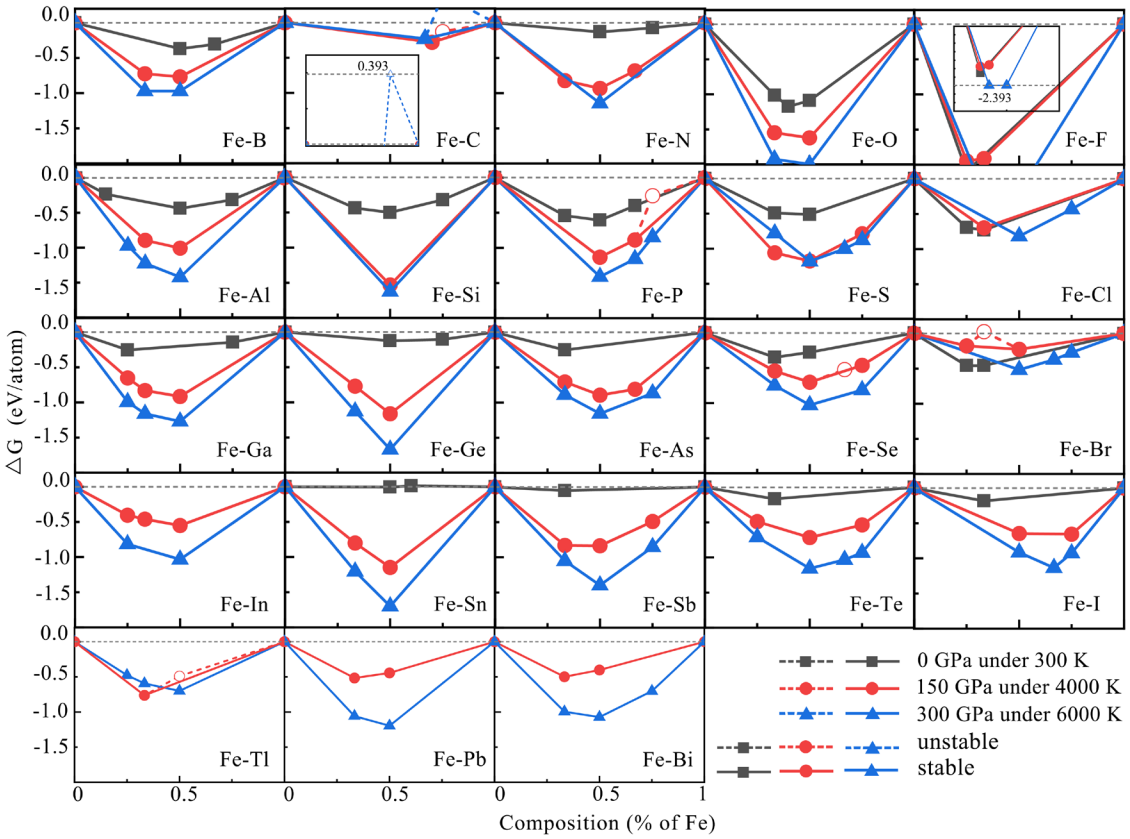
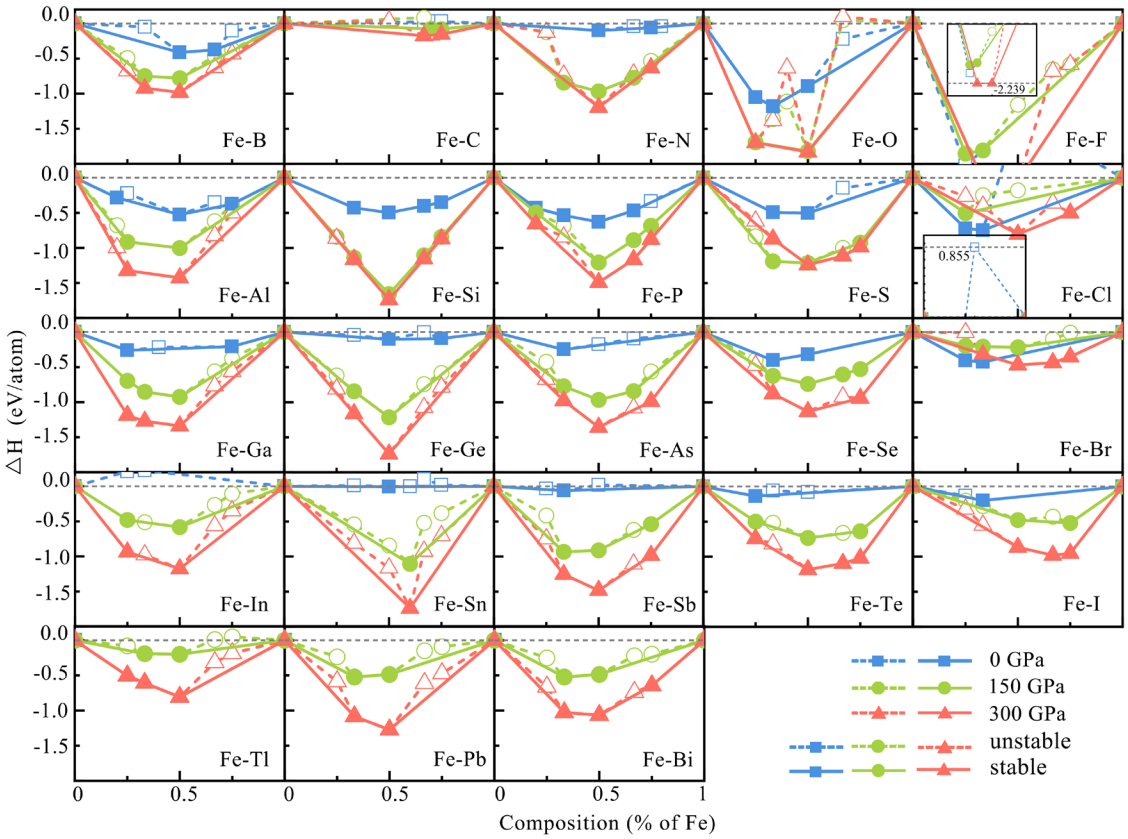
Details of DFT calculation

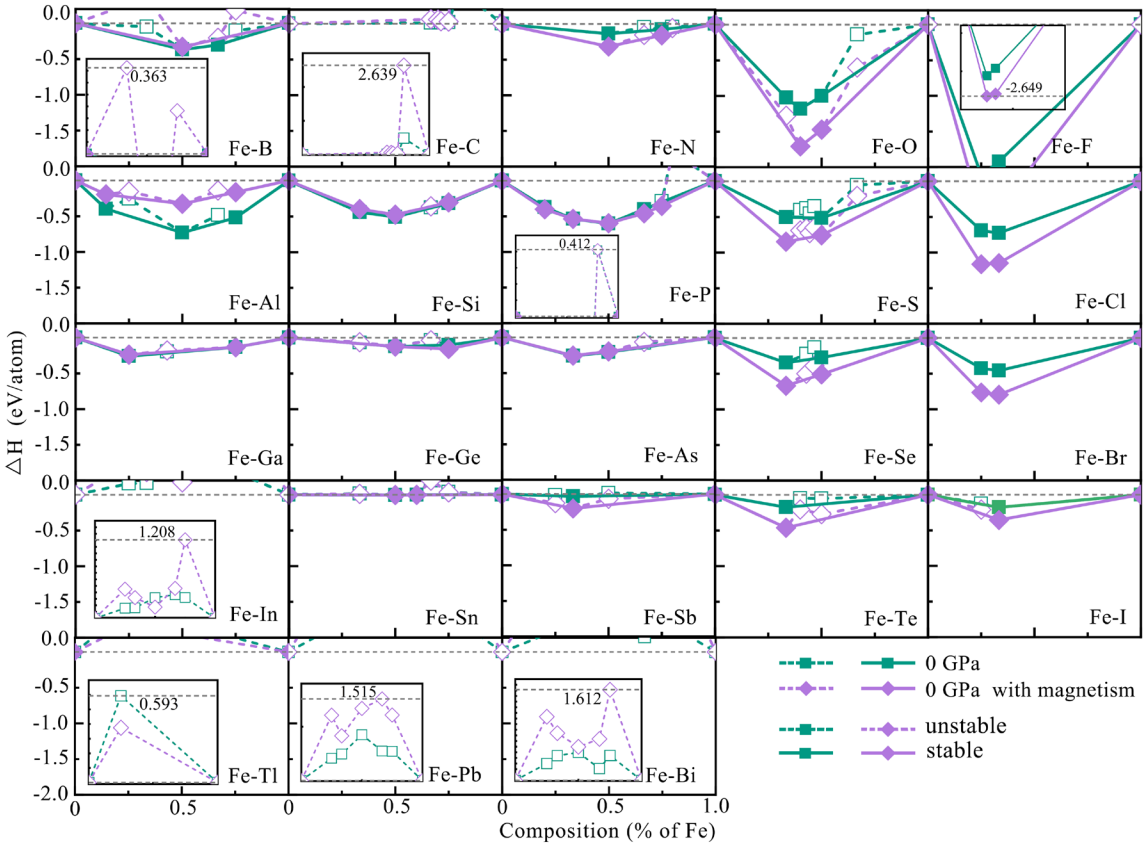
In the PAW potential, the following electrons are treated as valence, Fe: $3d^6 4s^2$, B: $2s^2 2p^1$, Al: $3s^2 3p^1$, Ga: $4s^2 4p^1$, In: $5s^2 5p^1$, Tl: $6s^2 6p^1$, C: $2s^2 2p^2$, Si: $3s^2 3p^2$, Ge: $4s^2 4p^2$, Sn: $5s^2 5p^2$, Pb: $6s^2 6p^2$, N: $2s^2 2p^3$, P: $3s^2 3p^3$, As: $4s^2 4p^3$, Sb: $5s^2 5p^3$, Bi: $6s^2 6p^3$, O: $2s^2 2p^4$, S: $3s^2 3p^4$, Se: $4s^2 4p^4$, Te: $5s^2 5p^4$, F: $2s^2 2p^5$, Cl: $3s^2 3p^5$, Br: $4s^2 4p^5$, I: $5s^2 5p^5$.



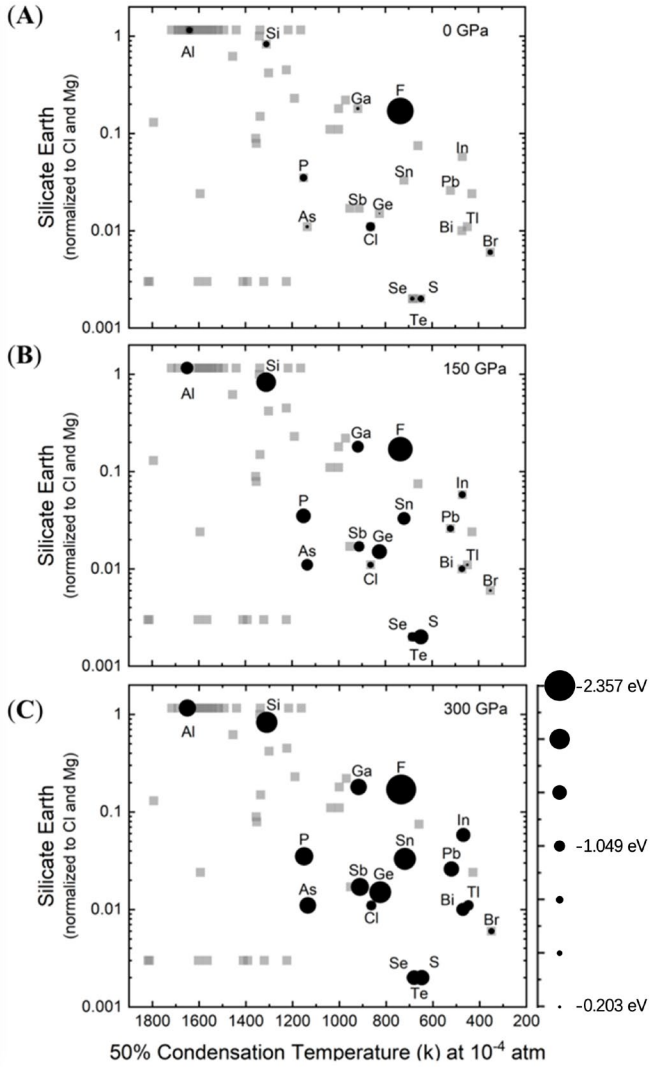
Supplementary Fig. 1. Formation energy (ΔG) considering the influence of temperature of main *p*-block – iron compounds at both ambient and high pressures. After the thermodynamic stability of these P-block elements was confirmed, we further considered the formation energy of the thermodynamically stable compounds under the influence of temperature to simulate their thermodynamic stability in actual conditions. Among them, 0 GPa and 300 K simulate the environment at the surface of the Earth's crust, 150 GPa and 4000 K simulate the environment in the mantle, and 300 GPa and 6000 K simulate the environment at the core-mantle boundary. Convex hulls are shown as solid lines, with stable compounds shown by solid symbols. Unstable compounds (open symbols) sit above convex hulls, with dotted lines indicating possible decomposition routes.



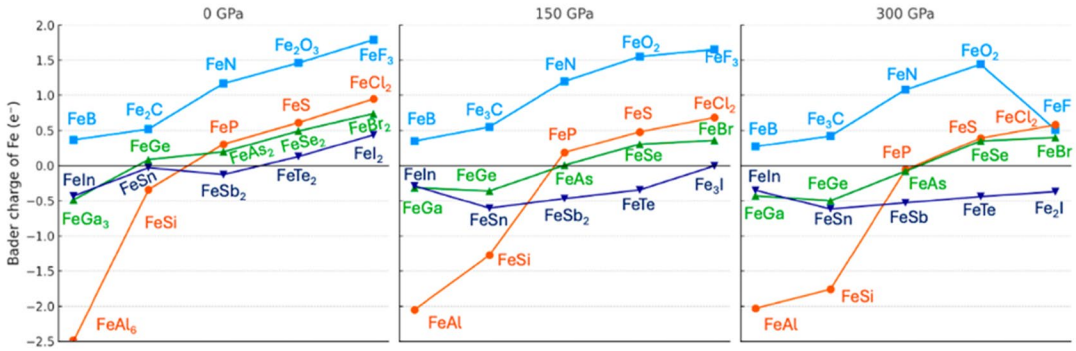
Supplementary Fig. 2. Thermodynamic stability of main *p*-block – iron compounds obtained by HSE calculations. Convex hulls are shown as solid lines, with stable compounds shown by solid symbols. Unstable compounds (open symbols) sit above convex hulls, with dotted lines indicating possible decomposition routes.



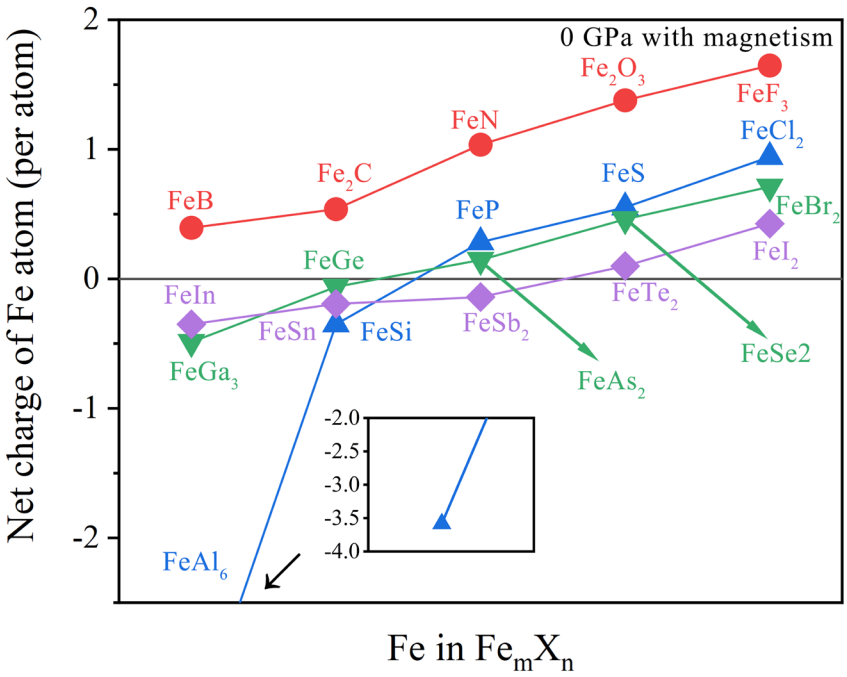
Supplementary Fig. 3. Effect of magnetism to the thermostability of Fe-X compounds under 0 GPa. Convex hulls are shown as solid lines, with stable compounds shown by solid symbols. Unstable compounds (open symbols) sit above convex hulls, with dotted lines indicating possible decomposition routes. The green lines with squares and the purple lines with circles show results of Fe-X in non-magnetic and ferromagnetic states. The magnetism is fully suppressed under 150 and 300 GPa, and therefore their comparison with nonmagnetic results is omitted. Under 0 GPa, the magnetism lowers the formation energies of some Fe-X compounds, but does not change the convexity of the hull. Therefore, it does not affect the thermodynamic stability of the Fe-X compounds.



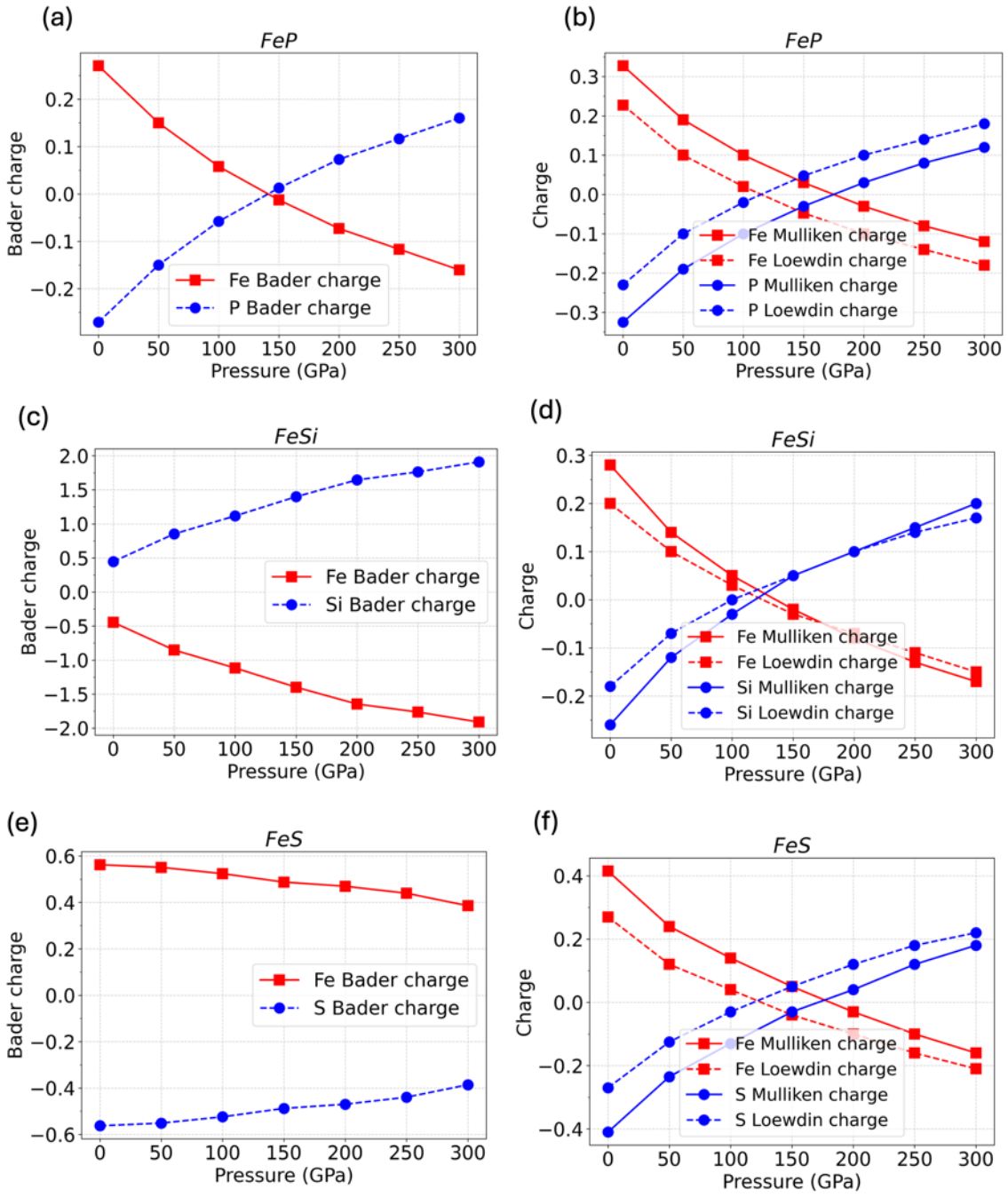
Supplementary Fig. 4. The abundance of elements in the Silicate Earth versus the binding strength with Fe. Electron Reproduction of a plot of the abundance of elements in the Silicate Earth (normalized to Mg and CI chondrites) versus their 50% condensation temperature at 10^{-4} atm. The size of the filled circles represents the binding strength of the element with Fe quantized by the enthalpy of formation per atom (larger symbols represent higher/lower binding strength). Three panels show three different pressures, 0, 150 and 300 GPa.



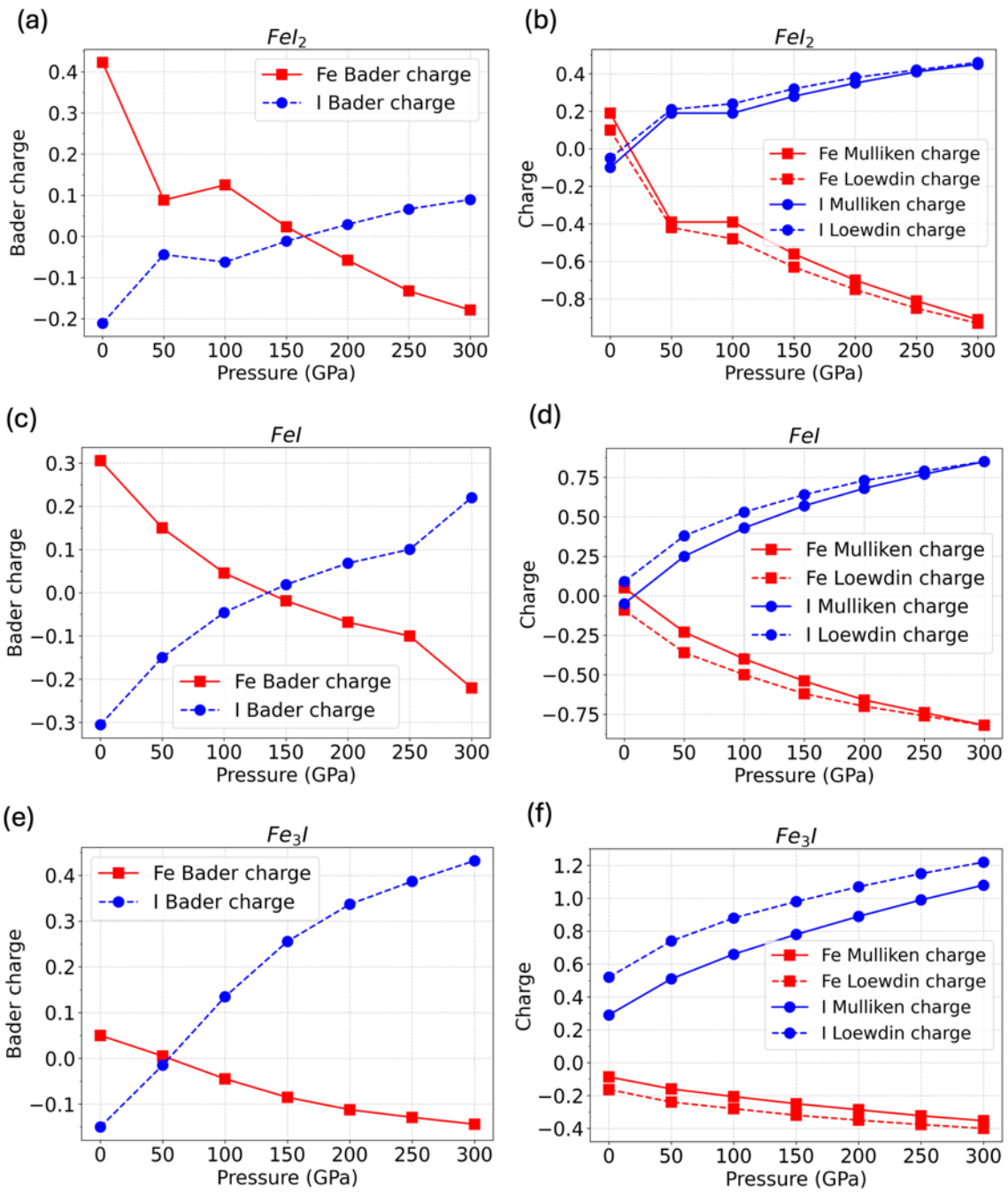
Supplementary Fig. 5. Bader charge of iron in Fe – *X* compounds at 0, 150 and 300 GPa, obtained using HSE hybrid functional.



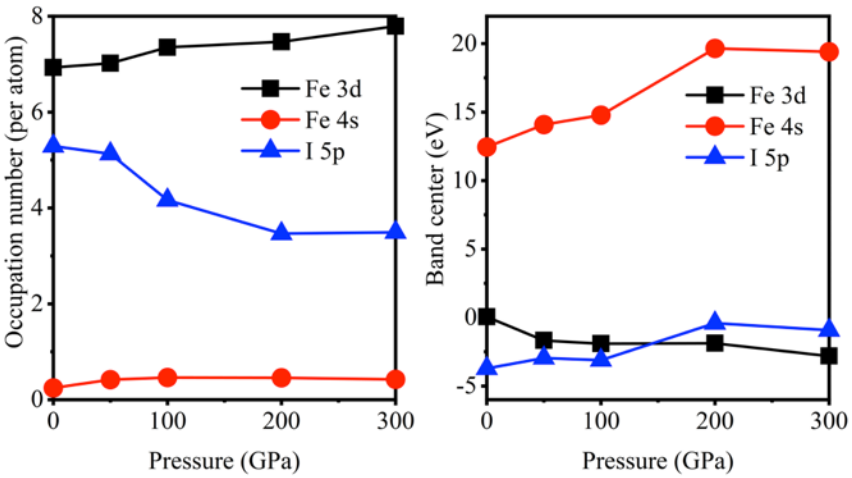
Supplementary Fig. 6. Bader charge of iron in Fe – *X* compounds at 0, 150 and 300 GPa with spin polarization. The magnetism is fully compressed under pressures of 150 and 300 GPa.



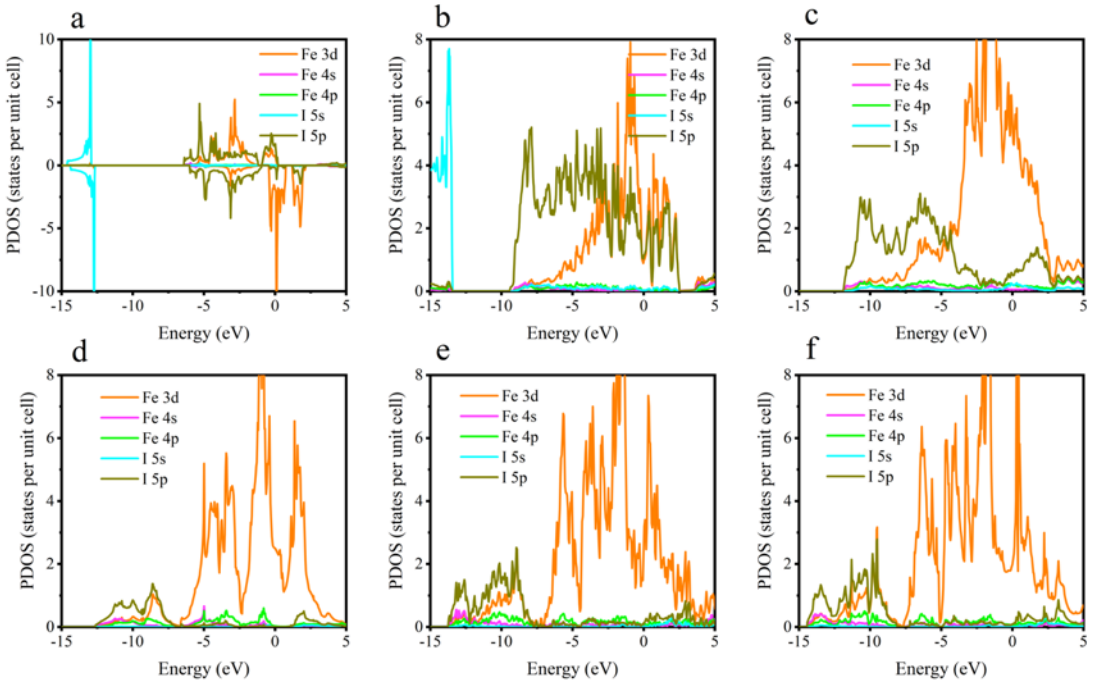
Supplementary Fig. 7. Comparing the Bader charges with the Mulliken and Löwdin charges. (a) The Bader charges for FeP from 0 to 300 GPa. (b) The Mulliken and Löwdin charges for FeP from 0 to 300 GPa. (c) and (d) The Bader, Mulliken and Löwdin charges for FeSi from 0 to 300 GPa. (e) and (f) The Bader, Mulliken and Löwdin charges for FeS from 0 to 300 GPa. The results obtained by different charge attribution partitioning methods show the same trend.



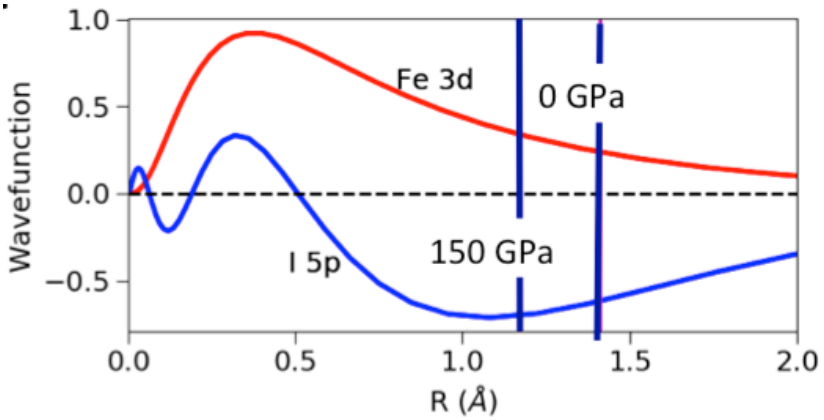
Supplementary Fig. 8. Comparing the Bader charges with the Mulliken and Löwdin charges. (a) The Bader charges for FeI_2 from 0 to 300 GPa. (b) The Mulliken and Löwdin charges for FeI_2 from 0 to 300 GPa. (c) and (d) The Bader, Mulliken and Löwdin charges for FeI from 0 to 300 GPa. (e) and (f) The Bader, Mulliken and Löwdin charges for Fe_3I from 0 to 300 GPa.



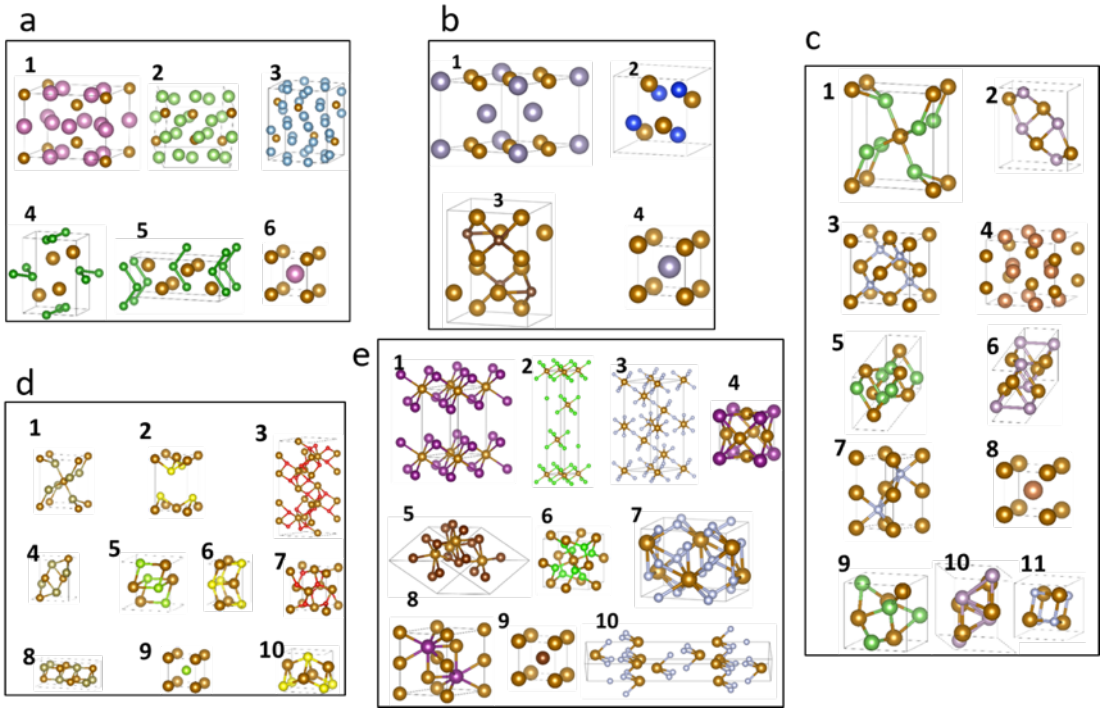
Supplementary Fig. 9. Occupation number and band center as function of pressure in Fe – I compounds. At each pressure, the compound that have the lowest enthalpy of formation per atom is chosen. The occupation numbers are calculated by projecting and integrating the wavefunctions to the atomic orbitals inside the Wigner-Seitz Radius. The band centers are calculated from the density of states (**Supplementary Fig. 10**) using the DOS analysis tool "dosanalyze.pl" in the VTST tool package from UT Austin.



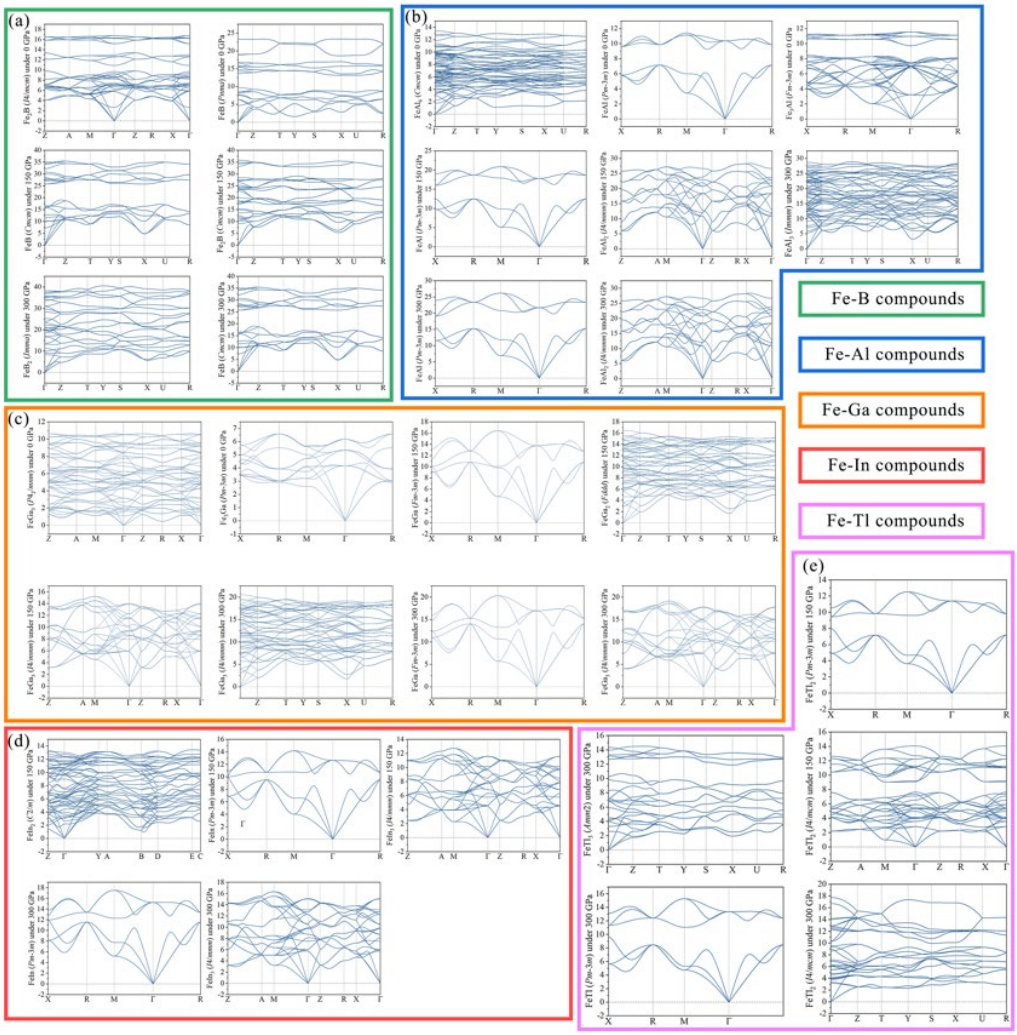
Supplementary Fig. 10. Electronic structures of Fe – I compounds. The projected DOS spectra of **a** FeI_2 with *P*-3*m*1 structure at 0 GPa; **b** FeI_3 with *R*-3 structure at 0 GPa; **c** FeI_3 with *R*32 structure at 50 GPa; **d** FeI with *P*-1 structure at 100 GPa; **e** Fe_3I with *Pm*-3*m* structure at 200 GPa; **f** Fe_2I with $P6_3/mmc$ structure at 400 GPa.



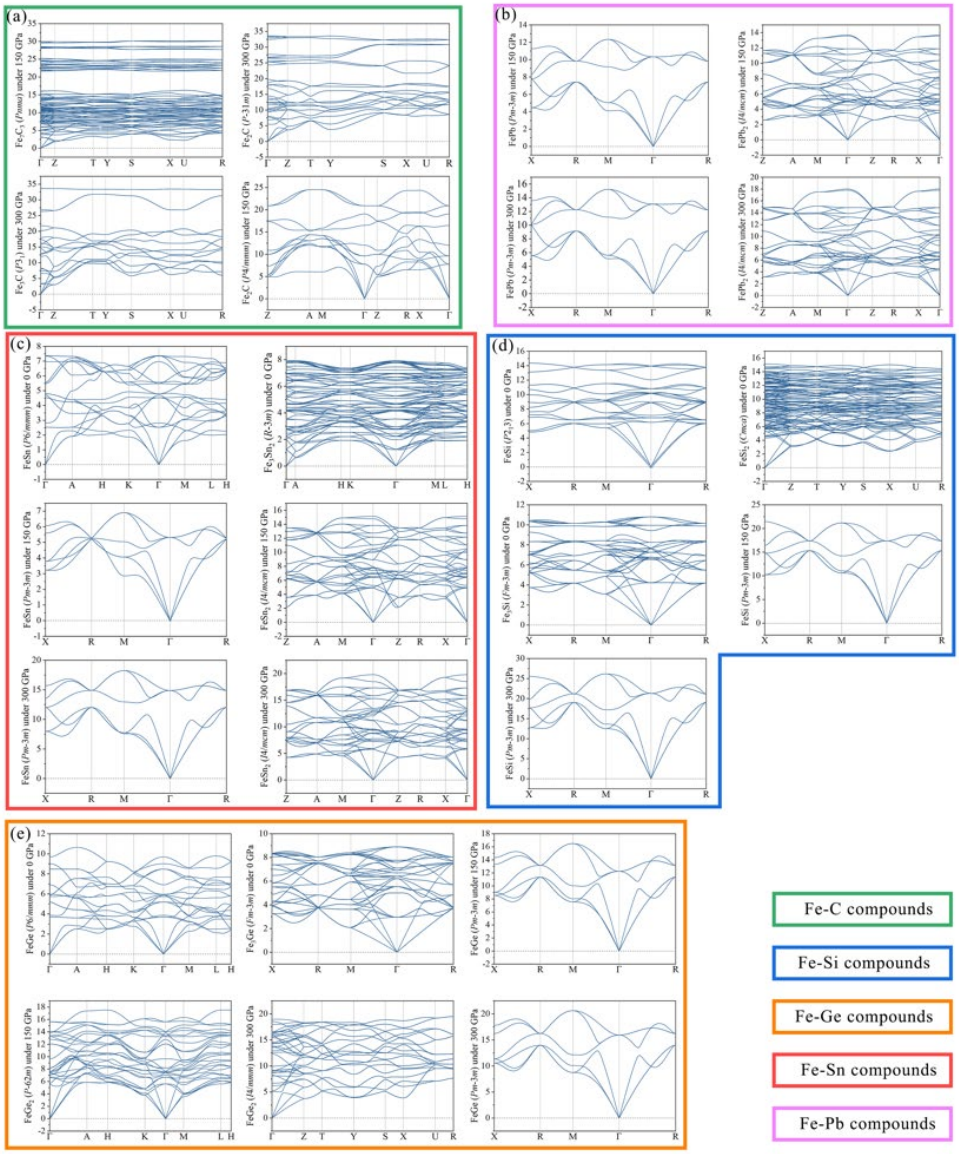
Supplementary Fig. 11. The free-atom wavefunctions of the iron 3*d* and Iodine 5*p* orbitals. The wavefunctions are calculated by use of the Fritz-Harber-Institute (FHI) pseudopotential generation package. The two vertical lines show the radii that are half of the Fe-I distances at 0 GPa and 150 GPa in the Fe-I compounds that have the lowest enthalpy of formation per atom at that pressure. It clearly shows that the compression of the compounds interferes much more significantly with iodine 5*p* orbitals than with Fe 3*d* orbitals. Therefore, the energy levels of iodine 5*p* will increase much faster with pressure than that of iron 3*d*, which is the driving force of the charge transfer reversal in Fe-I compounds under pressure.



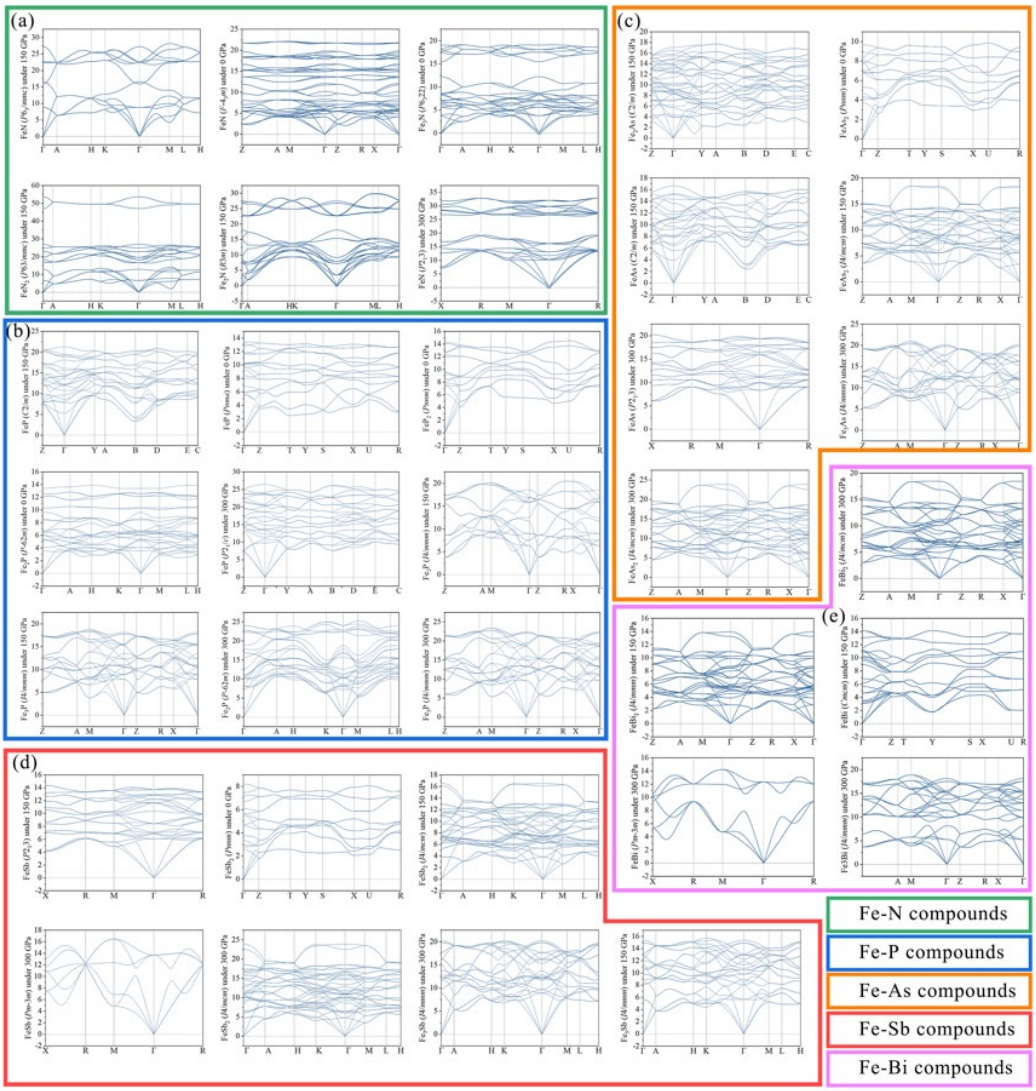
Supplementary Fig. 12. More crystal structures of Fe compounds with *p* elements, at 0 GPa, 150 GPa and 300 GPa. **a.** 1, $FeIn_3$ with *P*4 space group under 0 GPa; 2, $FeGa_3$ with $P4_2/mnm$ space group under 0 GPa; 3, $FeAl_6$ with *Cmcm* space group under 0 GPa; 4, FeB with *Pnma* space group under 0 GPa; 5, FeB with *Cmcm* space group under 150 GPa or 300 GPa; 6, FeIn, FeGa and FeAl with *Pm*-3*m* space group under 150 or 300 GPa. **b.** 1, FeSn and FeGe with *P*6/*mmm* space group under 0 GPa; 2, FeSi with $P2_13$ space group under 0 GPa; 3, Fe_3C with *Pnma* space group under 0 GPa, 150 GPa or 300 GPa; 4, FeSn, FeGe and FeSi with *Pm*-3*m* space group under 150 GPa or 300 GPa. **c.** 1, $FeSb_2$ and $FeAs_2$ with *Pnnm* space group under 0 GPa; 2, FeP with *Pnma* space group under 0 GPa; 3, FeN with *F*-43*m* space group under 0 GPa; 4, $FeSb_2$ with *I*4/*mcm* space group under 150 GPa; 5, FeAs with *C*2/*m* space group under 150 GPa; 6, FeP with *C*2/*m* space group under 150 GPa; 7, FeN with $P6_3/mmc$ space group under 150 GPa; 8, FeSb with *Pm*-3*m* space group under 300 GPa; 9, FeAs with $P2_13$ space group under 300 GPa; 10, FeP with $P2_1/c$ space group under 300 GPa; 11, FeN with $P2_13$ space group under 300 GPa. **d.** 1, $FeTe_2$ and $FeSe_2$ with *Pnnm* space group under 0 GPa; 2, FeS with *P*4/*nmm* space group under 0 GPa; 3, Fe_2O_3 with *R*-3*c* space group under 0 GPa; 4, FeTe with Pnma space group under 150 GPa; 5, FeSe with *Pbcm* space group under 150 GPa; 6, FeS with *Pmmn* space group under 150 GPa; 7, FeO_2 with *Pa*-3 space group under 150 GPa or 300 GPa; 8, FeTe with Cccm space group under 300 GPa; 9, FeSe with *Pm*-3*m* space group under 300 GPa; 10, FeS with *Fmmm* space group under 300 GPa. **e.** 1, FeI_2 and $FeBr_2$ with *P*-3*m*1 space group under 0 GPa; 2, $FeCl_2$ with *R*-3*m* space group under 0 GPa; 3, FeF*3* with R-3c space group under 0 GPa; 4, Fe_3I with *Pm*-3*m* space group under 150 GPa; 5, FeBr with *P*-1 space group under 150 GPa; 6, $FeCl_2$ with *Pa*-3 space group under 150GPa; 7, FeF_3 with Cmcm space group under 150 GPa; 8, Fe_2I with $P6_3/mmc$ space group under 300 GPa; 9, FeBr and FeCl with *Pm*-3*m* space group under 300 GPa; 10, FeF with *R*-3*m* space group under 300 GPa.



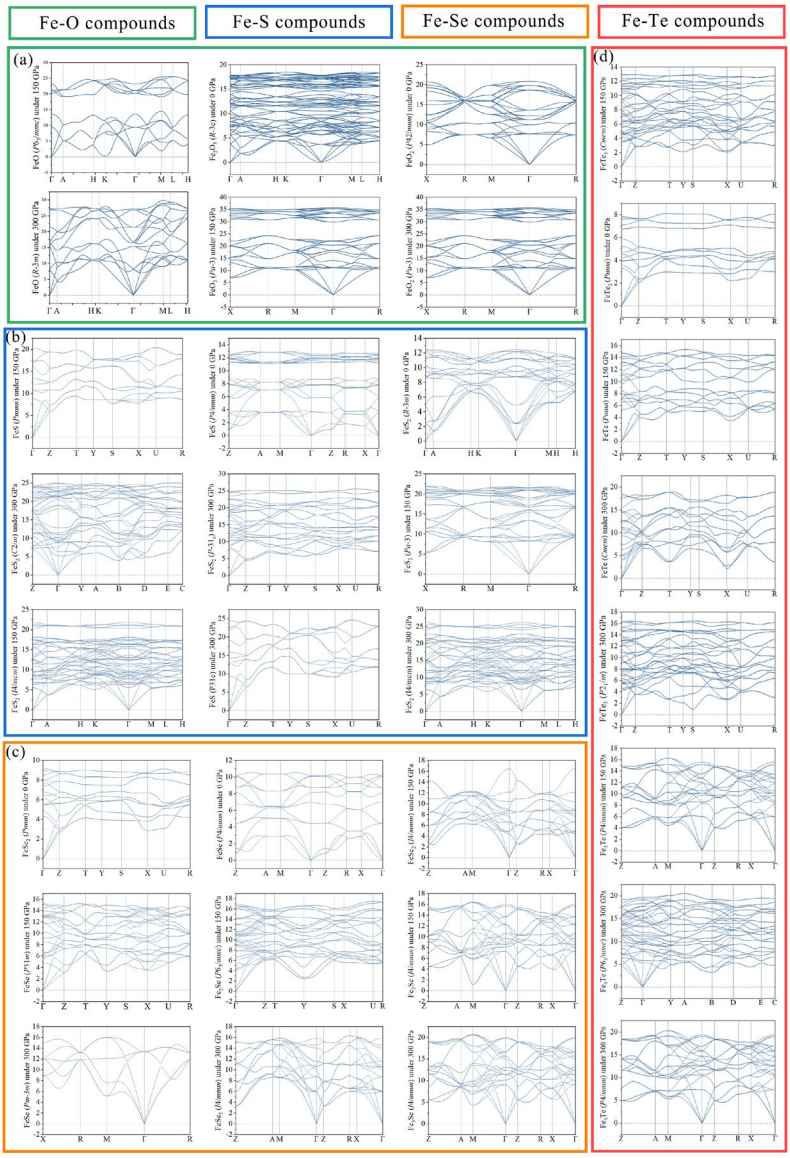
Supplementary Fig. 13. Dynamic stability of Fe-IIIA compounds. **a.** Phonon spectrum of Fe-B compounds, this includes: FeB (Pnma) under 0 GPa, Fe_2B (*I*4/*mcm*) under 0 GPa, FeB (*Cmcm*) under 150 GPa, Fe_2B (*Cmcm*) under 150 GPa, FeB_2 (*Imma*) under 300 GPa, FeB (*Cmcm*) under 300 GPa. **b.** Phonon spectrum of Fe-Al compounds, this includes: $FeAl_6$ (*Cmcm*) under 0 GPa, FeAl (*Pm*-3*m*) under 0 GPa, Fe_3Al (*Fm*-3*m*) under 0 GPa, $FeAl_3$ (*Immm*) under 300 GPa, FeAl (*Pm*-3*m*) under 150 GPa, $FeAl_2$ (*I*4/*mmm*) under 150 GPa, FeAl (*Pm*-3*m*) under 300 GPa, $FeAl_2$ (*I*4/*mmm*) under 300 GPa. **c.** Phonon spectrum of Fe-Ga compounds, this includes: $FeGa_3$ ($P4_2/mnm$) under 0 GPa, Fe_3Ga (*Pm*-3*m*) under 0 GPa, $FeGa_2$ (*Fddd*) under 150 GPa, FeGa (*Fm*-3*m*) under 150 GPa, $FeGa_3$ (*I*4/*mmm*) under 150 GPa, $FeGa_3$ (*I*4/*mmm*) under 300 GPa, FeGa (*Fm*-3*m*) under 300 GPa, $FeGa_3$ (*I*4/*mmm*) under 300 GPa. **d.** The phonon spectrum of Fe-In compounds, includes: $FeIn_2$ (*C*2/*m*) under 150 GPa, FeIn (*Pm*-3*m*) under 150 GPa, $FeIn_3$ (*I*4/*mmm*) under 150 GPa, FeIn (*Pm*-3*m*) under 300 GPa, $FeIn_3$ (*I*4/*mmm*) under 300 GPa. **e.** The phonon spectrum of Fe-Tl compounds, includes: $FeTl_3$ (*Amm*2) under 300 GPa, $FeTl_2$ (*Pm*-3*m*) under 150 GPa, $FeTl_2$ (*I*4/*mcm*) under 150 GPa, FeTl (*Pm*-3*m*) under 300 GPa, $FeTl_2$ (*I*4/*mcm*) under 300 GPa. The phonon spectra are calculated using finite displacement method by combining the features of phonopy (http://phonopy.sourceforge.net) and VASP programs.



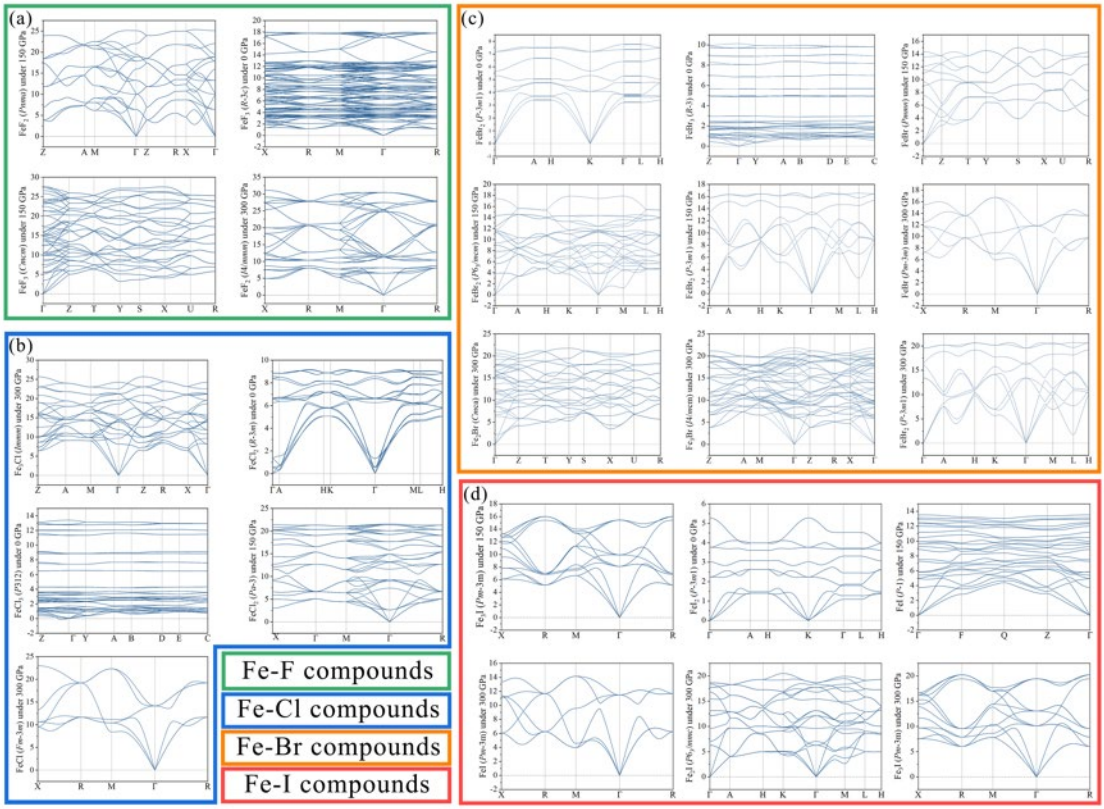
Supplementary Fig. 14. Dynamic stability of Fe–IVA compounds. **a.** The phonon spectrum of Fe-C compounds includes: Fe_7C_3 (*Pnma*) under 150 GPa, Fe_2C (*P*-31*m*) under 300 GPa, Fe_3C ($P3_1$) under 300 GPa, Fe_2C (*P*4/*mmm*) under 150 GPa. **b.** The phonon spectrum of Fe-Si compounds includes: $FeSi_2$ (*Cmca*) under 0 GPa, FeSi ($P2_13$) under 0 GPa, Fe_3Si (*Fm*-3*m*) under 0 GPa, FeSi (*Pm*-3*m*) under 150 GPa, FeSi (*Pm*-3*m*) under 300 GPa. **c.** The phonon spectrum of Fe-Ge compounds includes: FeGe (*P*6/*mmm*) under 0 GPa, Fe_3Ge (*Fm*-3*m*) under 0 GPa, FeGe (*Pm*-3*m*) under 150 GPa, $FeGe_2$ (*P*-62*m*) under 150 GPa, $FeGe_2$ (*I*4/*mmm*) under 300 GPa, FeGe (*Pm*-3*m*) under 300 GPa. **d.** The phonon spectrum of Fe-Sn compounds includes: FeSn (*P*6/*mmm*) under 0 GPa, Fe_3Sn_2 (*R*-3*m*) under 0 GPa, FeSn (*Pm*-3*m*) under 150 GPa, $FeSn_2$ (*I*4/*mcm*) under 150 GPa, FeSn (*Pm*-3*m*) under 300 GPa, $FeSn_2$ (*I*4/*mcm*) under 300 GPa. **e.** The phonon spectrum of Fe-Pb compounds includes: FePb (*Pm*-3*m*) under 150 GPa, $FePb_2$ (*I*4/*mcm*) under 150 GPa, FePb (*Pm*-3*m*) under 300 GPa, $FePb_2$ (*I*4/*mcm*) under 300 GPa.



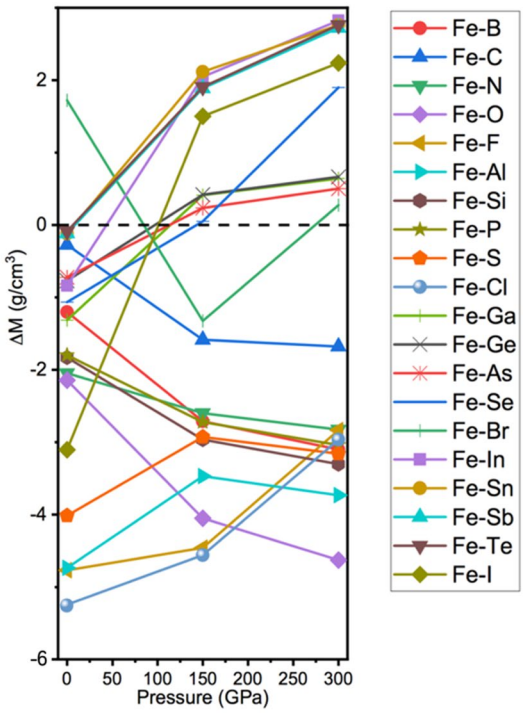
Supplementary Fig. 15. Dynamic stability of Fe–VA compounds. **a.** The phonon spectrum of Fe-N compounds includes: FeN (F-4$_3m$) under 0 GPa, Fe3N ($P6_322$) under 0 GPa, FeN ($P6_3/mmc$) under 150 GPa, FeN_2 (P6$_3$/mmc) under 150 GPa, Fe_2N ($R3m$) under 150 GPa, FeN (P2$_1$3) under 300 GPa. **b.** The phonon spectrum of Fe-P compounds includes: FeP ($Pnma$) under 0 GPa, FeP_2 ($Pnnm$) under 0 GPa, Fe_2P (P-62m) under 0 GPa, FeP ($C2/m$) under 150 GPa, FeP ($P2_1/c$) under 300 GPa, Fe_2P ($I4/mmm$) under 150 GPa, Fe_3P ($I4/mmm$) under 150 GPa, Fe_2P (P-62m) under 300 GPa, Fe_3P ($I4/mmm$) under 300 GPa. **c.** The phonon spectrum of Fe-As compounds includes: $FeAs_2$ ($Pnnm$) under 0 GPa, FeAs ($C2/m$) under 150 GPa, Fe_2As ($C2/m$) under 150 GPa, $FeAs_2$ ($I4/mcm$) under 150 GPa, FeAs ($P2_13$) under 300 GPa, Fe_3As ($I4/mmm$) under 300 GPa, $FeAs_2$ ($I4/mcm$) under 300 GPa. **d.** The phonon spectrum of Fe-Sb compounds includes: $FeSb_2$ ($Pnnm$) under 0 GPa, FeSb ($P2_13$) under 150 GPa, $FeSb_2$ ($I4/mcm$) under 150 GPa, Fe_3Sb ($I4/mmm$) under 150 GPa, FeSb (Pm-3m) under 300 GPa, $FeSb_2$ ($I4/mcm$) under 300 GPa, Fe_3Sb ($I4/mmm$) under 300 GPa. **e.** The phonon spectrum of Fe-Bi compounds includes: FeBi ($Cmcm$) under 150 GPa, $FeBi_2$ ($I4/mmm$) under 150 GPa, FeBi (Pm-3m) under 300 GPa, Fe_3Bi ($I4/mmm$) under 300 GPa, $FeBi_2$ ($I4/mcm$) under 300 GPa.



Supplementary Fig. 16. Dynamic stability of Fe–VIA compounds. **a.** The phonon spectrum of Fe-O compounds includes: FeO_2 ($P4_2/mnm$) under 0 GPa, Fe_2O_3 (R-3c) under 0 GPa, FeO_2 (Pa-3) under 150 GPa, FeO_2 (Pa-3) under 300 GPa. **b.** The phonon spectrum of Fe-S compounds includes: FeS ($P4/nmm$) under 0 GPa, FeS_2 (R-3m) under 0 GPa, FeS ($Pmmn$) under 150 GPa, FeS_2 ($C2/m$) under 300 GPa, FeS_2 (P-31c) under 300 GPa, FeS_2 (Pa-3) under 150 GPa, FeS_2 ($I4/mcm$) under 150 GPa, FeS ($P31c$) under 300 GPa, FeS_2 ($I4/mcm$) under 300 GPa. **c.** The phonon spectrum of Fe-Se compounds includes: $FeSe_2$ ($Pnnm$) under 0 GPa, FeSe ($P4/nmm$) under 0 GPa, FeSe ($P31m$) under 150 GPa, FeSe*2* ($I4/mmm$) under 150 GPa, Fe2Se (P63/mmc) under 150 GPa, Fe_3Se ($I4/mmm$) under 150 GPa, FeSe (Pm-3m) under 300 GPa, $FeSe_2$ ($I4/mmm$) under 300 GPa, Fe_3Se ($I4/mmm$) under 300 GPa. **d.** The phonon spectrum of Fe-Te compounds includes: $FeTe_2$ ($Pnnm$) under 0 GPa, FeTe ($Pnma$) under 150 GPa, $FeTe_3$ ($Cmcm$) under 150 GPa, FeTe ($Cmcm$) under 300 GPa, FeTe*3* ($P2_1/m$) under 300 GPa, Fe_3Te ($P4/mmm$) under 150 GPa, Fe_3Te ($P6_3/mmc$) under 300 GPa, Fe_3Te ($P4/mmm$) under 300 GPa.



Supplementary Fig. 17. Dynamic stability of Fe–VIIA compounds. **a.** The phonon spectrum of Fe-F compounds includes: FeF_3 (*R*-3*c*) under 0 GPa, FeF_2 (*Pnma*) under 150 GPa, FeF_3 (*Cmcm*) under 150 GPa, FeF_2 (*I*4/*mmm*) under 300 GPa. **b.** The phonon spectrum of Fe-Cl compounds includes: $FeCl_2$ (*R*-3*m*) under 0 GPa, $FeCl_3$ (*P*312) under 0 GPa, Fe_3Cl (*Immm*) under 300 GPa, $FeCl_2$ (*Pa*-3) under 150 GPa, FeCl (*Fm*-3*m*) under 300 GPa. **c.** The phonon spectrum of Fe-Br compounds includes: $FeBr_2$ (*P*-3*m*1) under 0 GPa, $FeBr_3$ (*R*-3) under 0 GPa, FeBr (*Pmmn*) under 150 GPa, Fe_2Br (*Cmca*) under 300 GPa, $FeBr_2$ ($P6_3/mcm$) under 150 GPa, FeBr (*Pm*-3*m*) under 300 GPa, Fe_3Br (*I*4/*mcm*) under 300 GPa, $FeBr_2$ (*P*-3*m*1) under 150 GPa, $FeBr_2$ (*P*-3*m*1) under 300 GPa. **d.** The phonon spectrum of Fe-I compounds includes: FeI_2 (*P*-3*m*1) under 0 GPa, FeI (*P*-1) under 150 GPa, Fe_3I (*Pm*-3*m*) under 150 GPa, FeI (*Pm*-3*m*) under 300 GPa, Fe_2I ($P6_3/mmc$) under 300 GPa, Fe_3I (*Pm*-3*m*) under 300 GPa.



Supplementary Fig. 18. Density difference between Fe_mX_n compounds and pure Fe. The density difference between Fe_mX_n (X= *p* elements) compounds and pure Fe at 0 GPa, 150 GPa and 300 GPa.

Supplementary Table 1. Structure information of all the structures reported in this work. Lattice and atomic position parameters of the structures of Fe-X compounds found by PSO structure search method.

Space group	Fe – X group (Pressure)	Lattice Parameters (Å)	Atom	Site	Atomic Positions		
Pnma (62)	FeP (0 GPa)	a=5.144; b=3.063;c=5.751 α=β=γ=90°	Fe P	4c 4c	0.50 0.69	0.25 0.25	0.70 0.07
	FeTe (150 GPa)	a=5.068; b=3.462;c=4.994 α=β=γ=90°	Fe Te	4c 4c	- 0.02 0.31	0.25 0.25	0.82 0.12
Cmcm (63)	FeB (150 GPa)	a=2.405; b=6.826; c=2.902 α=β=γ=90°	Fe B	4c 4c	0.00 0.00	0.36 0.08	0.25 0.25
	FeF_3 (150 GPa)	a=5.437; b=4.334; c=4.144 α=β=γ=90°	Fe F F	4c 4c 8e	0.00 0.00 0.79	0.74 0.32 0.00	0.25 0.25 0.00
	$FeAl_6$ (0 GPa)	a=7.429; b=6.474; c=8.778 α=β=γ=90°	Al Al Al Fe	8e 8f 8g 4c	0.68 0.00 0.32 0.00	0.00 0.15 0.29 0.46	0.00 0.40 0.25 0.25
	FeTe (300 GPa)	a=2.574; b=8.228; c=3.490 α=β=γ=90°	Fe Te	4c 4c	0.00 0.00	0.59 0.85	0.25 0.25
Pnnm (58)	Fe_2C (0 GPa)	a=4.709; b=4.279; c=2.822 α=β=γ=90°	Fe C	4g 2d	0.16 0.00	0.25 0.50	0.00 0.50
	$FeAs_2$ (0 GPa)	a=5.990; b=5.309; c=2.888 α=β=γ=90°	Fe As	2b 4g	0.00 0.86	0.00 0.32	0.50 0.00
	$FeSe_2$ (0 GPa)	a=5.782; b=4.807; c=3.600 α=β=γ=90°	Fe Se	2b 4g	0.00 0.87	0.00 0.28	0.50 0.00
	$FeSb_2$ (0 GPa)	a=6.519; b=5.768; c=3.287 α=β=γ=90°	Fe Sb	2b 4g	0.00 0.86	0.00 0.30	0.50 0.00
	$FeTe_2$ (0 GPa)	a=6.254; b=5.255; c=3.892 α=β=γ=90°	Fe Te	2b 4g	0.00 0.86	0.00 0.27	0.50 0.00
Cmc2_1 (36)	Fe_2C (150 GPa)	a=2.314; b=7.997; c=4.262 α=β=γ=90°	Fe Fe C	4a 4a 4a	0.00 0.00 0.00	0.71 0.03 0.38	0.66 - 0.04 0.76
*I*4/*mcm* (140)	Fe_2C (300 GPa)	a= b=4.286; c=3.713 α=β=γ=90°	Fe C	8h 4a	0.17 0.00	0.67 0.00	0.00 0.25
	$FeSb_2$ (150 GPa)	a= b=5.437; c=4.843 α=β=γ=90°	Fe Sb	4a 8h	0.00 0.34	0.00 0.84	0.25 0.00
F-43*m* (216)	FeN (0 GPa)	a=b=c=4.233 α=β=γ=90°	Fe N	4a 4d	0.00 0.75	0.00 0.75	0.00 0.75
P6_3/*mmc* (194)	FeN (150 GPa)	a=b=2.505; c=4.540 α=β=90°;γ=120°	Fe N	2a 2d	0.00 0.33	0.00 0.67	0.00 0.75
	Fe_2I (400 GPa)	a=b=3.517; c=4.323 α=β=90°; γ=120°	Fe Fe I	2d 2a 2c	0.33 0.00 0.33	0.67 0.00 0.67	0.75 0.00 0.25

*P*2$_1$3 (198)	FeN (300 GPa)	a=b=c=3.492 α=β=γ=90°	Fe N	4a 4a	0.80 0.20	0.80 0.20	0.80 0.20
	FeSi (0 GPa)	a=b=c=4.449 α=β=γ=90°	Fe Si	4a 4a	0.14 0.84	0.14 0.84	0.14 0.84
	FeAs (300 GPa)	a=b=c=3.938 α=β=γ=90°	Fe As	4a 4a	0.40 0.09	0.40 0.09	0.40 0.09
R-3*c* (167)	Fe_2O_3 (0 GPa)	a=b=4.780; c=13.361 α=β= 90°; γ=120°	Fe O	12c 18e	0.00 0.69	0.00 0.00	0.85 0.25
	FeF_3 (0 GPa)	a=b=5.296; c=13.561 α=β=90°; γ=120°	Fe F	6b 18e	0.00 0.59	0.00 0.00	0.00 0.25
	$FeBr_3$ (50 GPa)	a=b=5.140; c=13.334 α=β=90°; γ=120°	Fe Br	6b 18e	0.00 0.70	0.00 0.00	0.00 0.25
Pa-3 (205)	FeO_2 (150 GPa)	a=b=c=4.186 α=β=γ=90°	Fe O	4b 8c	0.50 0.13	0.50 0.13	0.50 0.13
*P*4$_2$/*mnm* (136)	FeF_2 (0 GPa)	a=b=4.798; c=3.342 α=β=γ=90°	Fe F	2a 4f	0.00 0.70	0.00 0.70	0.00 0.00
	$FeGa_3$ (0 GPa)	a=b=6.261; c=6.558 α=β=γ=90°	Ga Ga Fe	8j 4c 4f	0.34 0.00 0.84	0.34 0.50 0.84	0.26 0.00 0.00
R-3*m* (166)	FeF (300 GPa)	a=b=2.132; b=17.317 α=β=90°; γ=120°	Fe F	6c 6c	0.00 0.00	0.00 0.00	0.28 0.87
Pm-3*m* (221)	FeAl (150 GPa)	a=b=c=2.526	Al Fe	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
α=β=γ=90°	FeSi (150 GPa)	a=b=c=2.489	Fe Si	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeCl (300 GPa)	a=b=c=2.415	Cl Fe	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeGa (150 GPa)	a=b=c=2.561	Fe Ga	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeGe (150 GPa)	a=b=c=2.580	Fe Ge	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeSe (300 GPa)	a=b=c=2.500	Fe Se	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeBr (250 GPa)	a=b=c=2.603	Fe Br	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeIn (150 GPa)	a=b=c=2.722	Fe In	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	FeSn (150 GPa	a=b=c=2.738	Fe Sn	1b 1a	0.50 0.00	0.50 0.00	0.50 0.00
	$FeSb_2$ (300 GPa)	a=b=c=2.617	Fe Sb	1a 1b	0.00 0.50	0.00 0.50	0.00 0.50
	Fe_3I (150 GPa)	a=b=c=3.308	Fe I	3c 1a	0.00 0.00	0.50 0.00	0.50 0.00
*C*2/*m* (12)	FeP (150 GPa)	a=7.339; b=2.460; c=3.552 α=γ=90°; β=104°	Fe P	4i 4i	0.61 0.13	0.00 0.00	0.31 0.82
	$FeCl_3$ (150 GPa)	a=4.372; b=8.046; c=4.556 α=γ=90°;β=106°	Fe Cl Cl	4h 8j 4i	0.00 0.75 0.73	0.19 0.15 0.00	0.50 0.81 0.27

	FeAs (150 GPa)	a=7.697; b=2.583; c=3.674 α=γ=90°; β=103°	Fe As	4i 4i	0.11 0.62	0.00 0.00	0.81 0.31
*P*2$_1$/c (14)	FeP (300 GPa)	a=3.728; b=3.764; c=4.403 α=γ=90°; β=119°	Fe P	4e 4e	0.81 0.69	0.65 0.35	0.10 0.41
*P*4/*nmm* (129)	FeS (0 GPa)	a=b=3.592; c=5.458 α=β=γ=90°	Fe S	2a 2c	0.75 0.25	0.25 0.25	0.00 0.78
Pmmn (59)	FeS (150 GPa)	a=2.464; b=3.428; c=3.808 α=β=γ=90°	Fe S	2a 2b	0.25 0.25	0.36 0.14	0.25 0.75
R-3*m* (166)	$FeCl_2$ (0 GPa)	a=b=3.524; c=20.013 α=β=90°; γ=120°	Fe Cl	3a 6c	0.00 0.00	0.00 0.00	0.00 0.26
*P*312 (149)	$FeCl_3$ (0 GPa)	a=b=6.188; c=18.705 α=β=90°; γ=120°	Fe Fe Fe Fe Cl Cl Cl	2i 2g 1c 1e 6l 6l 6l	0.67 0.00 0.33 0.67 0.00 - 0.03 - 0.03	0.33 0.00 0.67 0.33 0.37 0.30 0.67	0.67 0.34 0.00 0.00 - 0.07 0.26 0.41
*P*6/*mmm* (191)	FeGe (0 GPa) FeSn (0 GPa)	a=b=4.963; c=4.057 α=β=90°; γ=120° a=b=5.292; c=4.459 α=β=90°; γ=120°	Fe Ge Ge Fe Sn Sn	3f 1a 2d 3f 1a 2d	0.50 0.00 0.33 0.50 0.00 0.33	0.00 0.00 0.67 0.00 0.00 0.67	0.00 0.00 0.50 0.00 0.00 0.50
Pbcm (57)	FeSe (150 GPa)	a=4.451; b=4.151; c=4.021 α=β=γ=90°	Fe Se	4d 4d	0.17 0.69	0.06 0.05	0.25 0.25
P-1 (2)	FeBr (150 GPa)	a=4.159; b=4.667; c=5.149 α=63°; β=73°; γ=89°	Fe Fe Br Br	2i 2i 2i 2i	0.15 0.65 0.83 0.33	0.75 0.45 0.68 0.05	0.79 0.79 0.28 0.28
P-3*m*1 (164)	$FeBr_2$ (0 GPa) FeI_2 (0 GPa)	a=b=3.217; c=4.044 α=β=90°; γ=120° a=b=4.013; c=7.288 α=β=90°; γ=120°	Fe Br Fe I	1a 2d 1a 2d	0.00 0.33 0.00 0.33	0.00 0.67 0.00 0.67	0.00 0.28 0.00 0.22
*P*4 (75)	FeIn (0 GPa)	a=b=7.123; c=5.366 α=β=γ=90°	Fe Fe Fe In In In	1a 1b 1b 1a 4d 4d	0.00 0.50 0.50 0.00 0.51 0.25	0.00 0.50 0.50 0.00 0.80 0.25	- 0.02 0.77 0.18 0.48 0.47 - 0.03