Supporting Information for Elastic properties of the pyrite-type FeOOH–AlOOH system from first principles calculations

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Equation S1.

$$\overline{C_{11}} = \frac{C_{11} + C_{22} + C_{33}}{3} \tag{1}$$

Equation S2.

$$\overline{C_{12}} = \frac{C_{12} + C_{13} + C_{23}}{3} \tag{2}$$

Equation S3.

$$\overline{C_{44}} = \frac{C_{44} + C_{55} + C_{66}}{3} \tag{3}$$

Equation S4.

$$AV_S = \frac{V_{Smax}(\vec{n}) - V_{Smin}(\vec{n})}{\langle V_S \rangle} \times 100 \tag{4}$$

Table S1. Lattice parameters (a, b, c) of pyrite-type FeO_2H and AlO_2H from 60 to 140 GPa.

P (GPa)	*Pbca* FeO_2H			*Pa*$\bar{3}$ FeO_2H	*Pa*$\bar{3}$ AlO_2H
	a (Å)	b (Å)	c (Å)	a (Å)	a (Å)
60	4.567	4.549	4.530	4.554	4.494
70	4.537	4.516	4.499	4.522	4.461
80	4.505	4.489	4.469	4.492	4.431
90	4.476	4.462	4.441	4.465	4.402
100	4.448	4.438	4.417	4.439	4.376
110	4.422	4.415	4.393	4.415	4.351
120	4.399	4.392	4.371	4.393	4.328
130	4.376	4.372	4.350	4.372	4.306
140	4.355	4.352	4.331	4.352	4.285

Table S2. Comparison of the elastic constants of pyrite-type FeO_2H and AlO_2H as a function of pressure (P) from 70 to 140 GPa. As the *Pbca* symmetry is orthorhombic, the C_{11}, C_{12}, and C_{44} for *Pbca* FeO_2H were obtained by averaging elements from the full, nine-constant elastic tensor using Equation S1-S3.

P	*Pbca* FeO_2H			*Pa*$\bar{3}$ FeO_2H			*Pa*$\bar{3}$ AlO_2H		
	$\overline{C_{11}}$	$\overline{C_{12}}$	$\overline{C_{44}}$	C_{11}	C_{12}	C_{44}	C_{11}	C_{12}	C_{44}
60	—	—	—	700	323	165	805	250	201
70	725	359	116	741	358	172	857	470	208
80	776	388	145	785	395	178	907	504	217
90	817	421	156	823	430	182	956	537	224
100	861	455	173	859	467	185	1004	570	232
110	900	489	179	894	502	188	1051	603	239
120	938	524	188	927	538	191	1097	635	247
130	975	558	197	963	573	194	1141	668	254
140	1011	592	206	992	610	197	1186	701	261

Table S3. Full elastic constant tensor of orthorhombic (*Pbca*) pyrite-type FeO_2H as a function of pressure (P) from 70 to 140 GPa.

P	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
70	709	365	344	740	369	727	176	80	93
80	750	391	385	796	388	783	185	123	129
90	790	423	421	837	419	823	192	128	149
100	831	461	457	879	448	873	204	150	165
110	865	496	492	918	481	918	210	159	169
120	899	531	526	956	513	960	217	166	181
130	930	566	561	993	546	1001	223	177	192
140	963	601	594	1030	580	1041	228	190	201

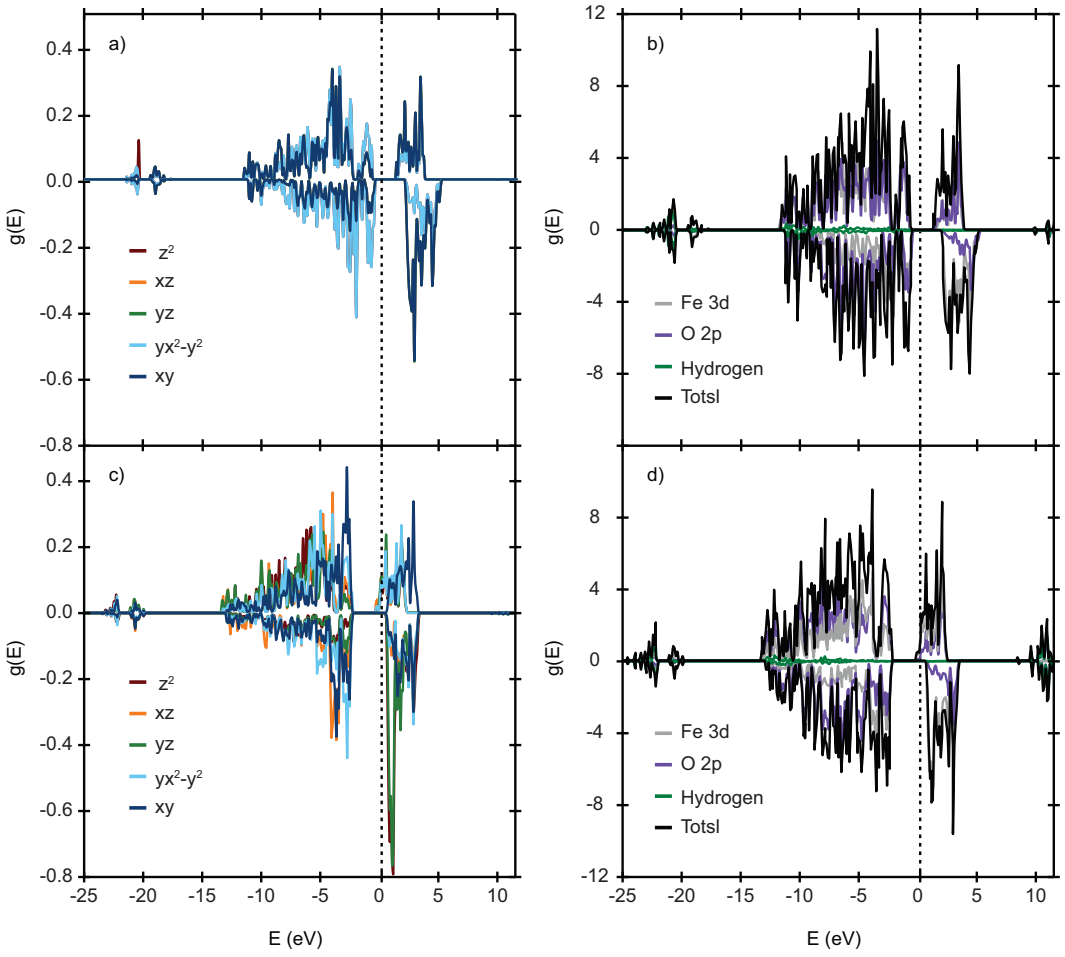

Figure S1. Calculated density of states (DOS) of the pyrite-type FeO_2H system at 100 GPa, for both the cubic $Pa\bar{3}$ structure (a, b) and the orthorhombic *Pbca* structure (c, d). The Fermi level (E_F) is indicated by a vertical dashed line. The slight overlap of the conduction band with E_F suggests that the *Pbca* structure is a semimetal or *n*-type semiconductor at this pressure.

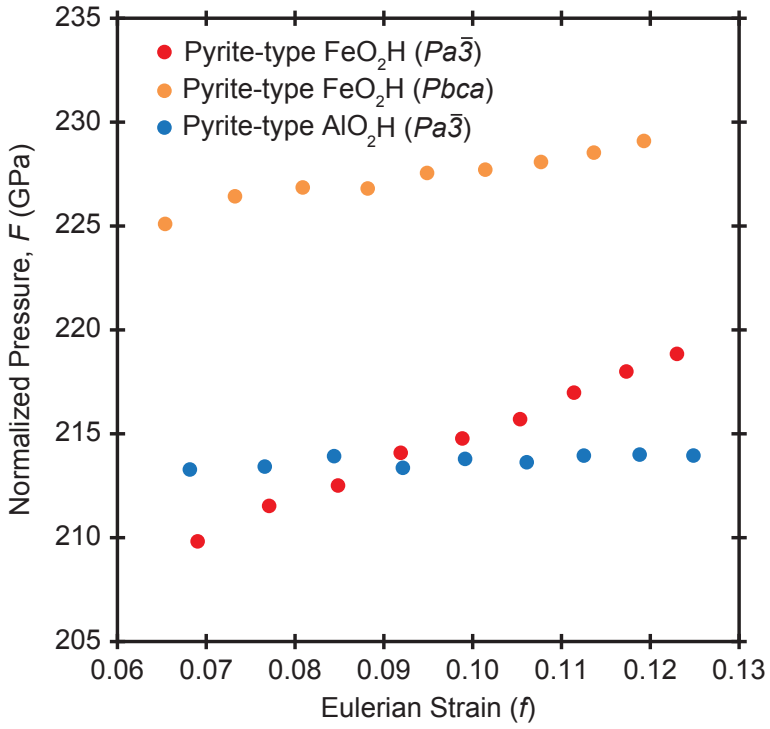

Figure S2. Eulerian strain (f) versus the normalized pressure (F) of $Pa\bar{3}$ FeO_2H, $Pbca$ FeO_2H, and $Pa\bar{3}$ AlO_2H, using V_0 values from lines 2, 5, and 7 of Table 1, respectively.