Supplemental material for

Stability of fcc phase FeH to 137 GPa

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FIGURE S1. Photo image of a sample at 107 GPa before laser heating. Diameter of the culet of the diamond anvil is 120 μm. Iron foil in the center of the sample space is surrounded by the transparent NaCl gasket and solid molecular hydrogen.

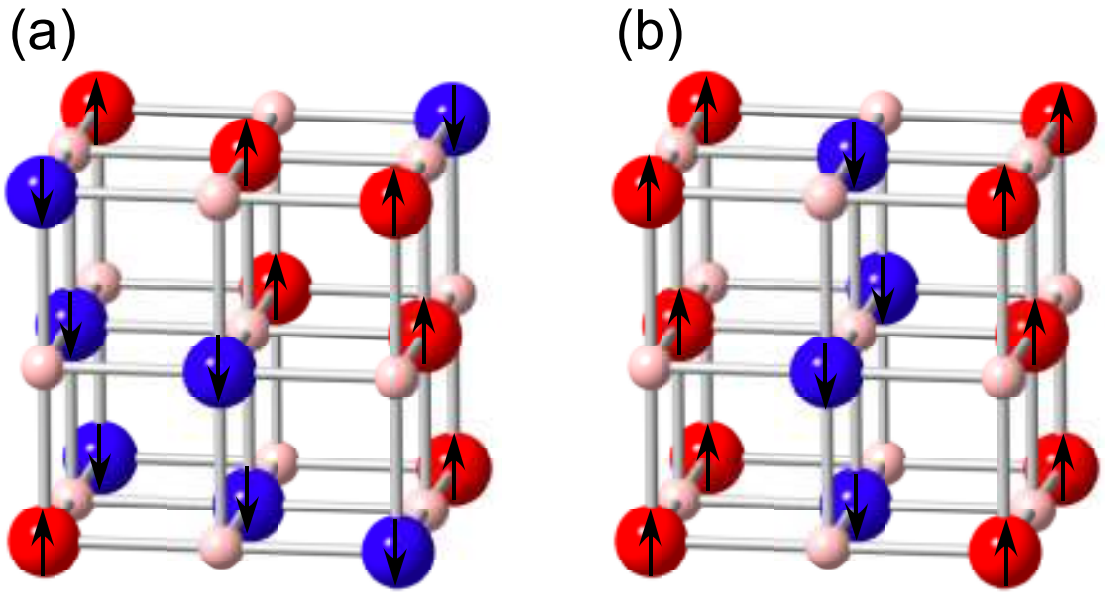

FIGURE S2. Two spin configurations of AFM FeH. Red and blue spheres denote iron atoms with up and down spins, respectively. White ones denote hydrogen atoms. Iron atoms on (a) the (111) plane or (b) the (100) plane have the same spin, and opposite spins occur on the adjacent planes.

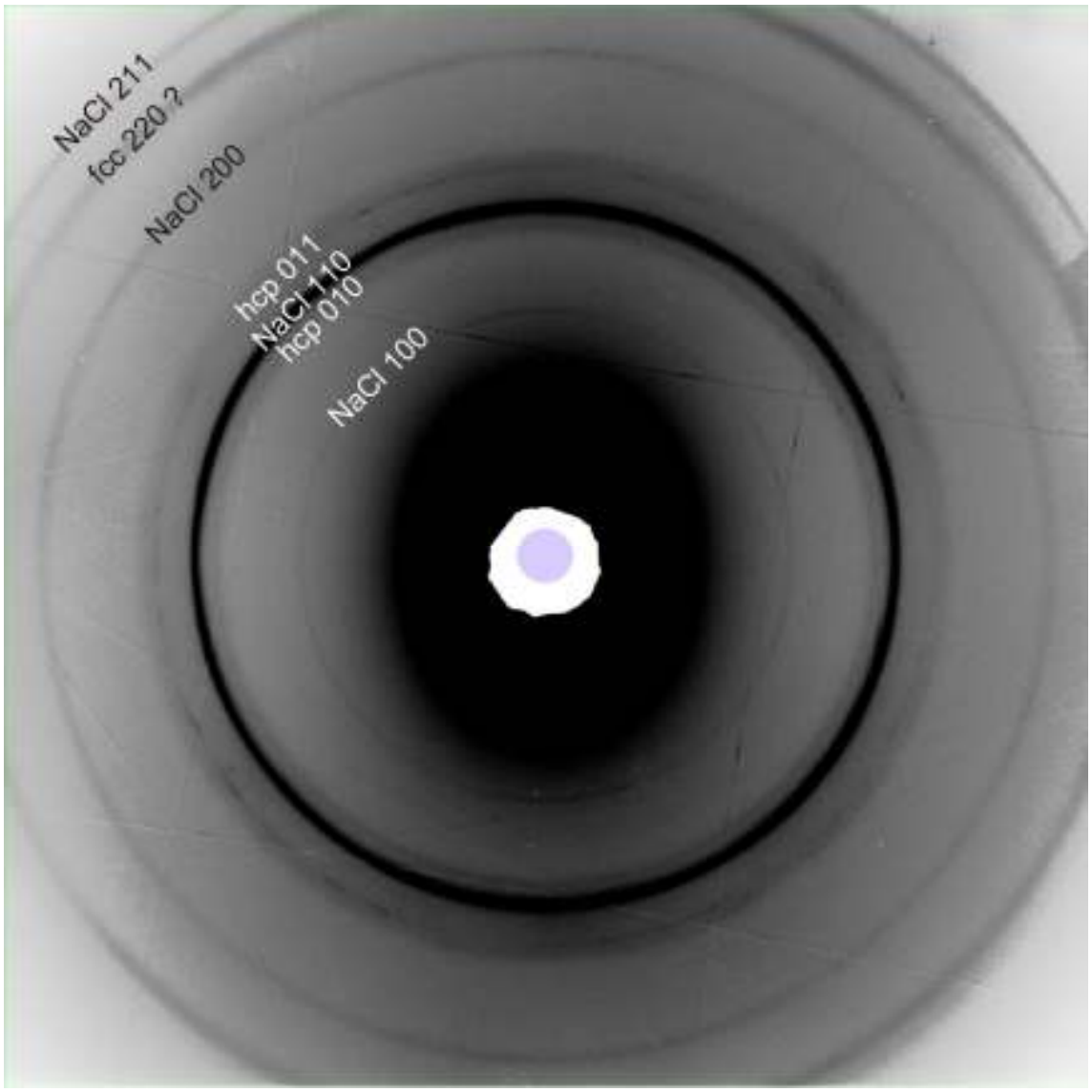

FIGURE S3. Two-dimensional XRD image corresponding to the middle pattern in Fig. 1a.

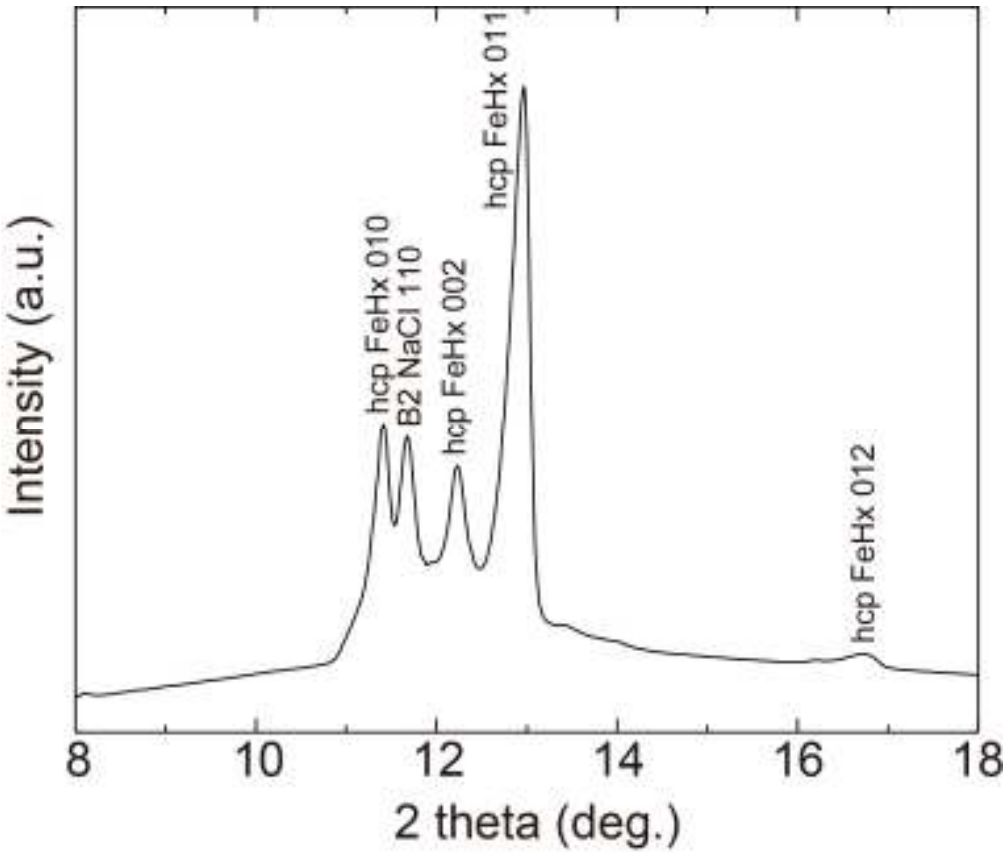

FIGURE S4. XRD pattern of hcp FeH_x obtained at 53 GPa after heating (Run #8).

TABLE S1. Experimental results of simultaneous measuremnets of lattice parameters of B2 NaCl and B2 KCl.

	B2 NaCl				B2 KCl			
Run#	a (Å)	a error (Å)	Pressure (GPa)	Pressure error (GPa)	a (Å)	a error (Å)	Pressure (GPa)	Pressure error (GPa)
1	2.90260	0.00028	51.76	0.06	3.10702	0.00066	52.13	0.14
2	2.79134	0.00079	82.32	0.26	2.98888	0.00100	83.01	0.32
3	2.73330	0.00036	103.73	0.15	2.92310	0.00123	106.65	0.49
4	2.70364	0.00024	116.48	0.11	2.88626	0.00035	122.46	0.16
5	2.66881	0.00605	133.24	3.09	2.83775	0.00002	146.60	0.01

TABLE S2. Summary of experimental condition s and observed phases.

Run#	Starting material	Pressure marker	Culet size (μm)	Pressure before heating (GPa)	Observed phase(s) before heating in order of dominance	Heating duration (min)	Peak temperature (K)	Pressure after heating (GPa)	Resultant phase assemblage in order of dominance
1	Fe, paraffin	Ruby	300	57.5	hcp-Fe	330	1770(100)	48.5	fcc-FeH_x, diamond
2	Fe, paraffin	KCl	120	68.7	hcp-Fe	65	1670(80)	62.9	fcc-FeH_x, diamond
3	Fe, paraffin	KCl	120	46.8	hcp-Fe	90	2060(220)	42.5	fcc-FeH_x
4	Fe, liquid H_2	NaCl	120	125.6	hcp-Fe	39	~1000	121.5	fcc-FeH_x, FeH_3
5	Fe, liquid H_2	NaCl	120	106.4	hcp-Fe	84	~1000	102.5	hcp-Fe, fcc-FeH_x
				102.5	hcp-Fe, fcc-FeH_x	53	~1000	98.5	fcc-FeH_x, FeH_3
				126.9	fcc-FeH_x	37	~1000	137.1	fcc-FeH_x
6	Fe, liquid H_2	NaCl	120	85.3	hcp-FeH_x	14	~1000	91.3	fcc-FeH_x, hcp-FeH_x
				92.4	fcc-FeH_x, hcp-FeH_x	31	~1000	99.3	fcc-FeH_x, hcp-FeH_x, FeH_2
				101.0	fcc-FeH_x, hcp-FeH_x, FeH_2	10	~1000	104.8	fcc-FeH_x, hcp-FeH_x, FeH_2
				76.9	fcc-FeH_x, hcp-FeH_x, FeH_2	9	~1000	71.6	fcc-FeH_x, hcp-FeH_x, FeH_2
				70.5	fcc-FeH_x, hcp-FeH_x, FeH_2	8	~1000	66.2	fcc-FeH_x, hcp-FeH_x, FeH_2
				56.7	fcc-FeH_x, hcp-FeH_x, FeH_2	4	~1000	54.6	fcc-FeH_x
				34.5	fcc-FeH_x	22	~1000	25.1	fcc-FeH_x, dhcp-FeH_x ($X<1$)?
7	Fe, liquid H_2	NaCl	120	69.7	dhcp-FeH_x	13	~1000	80.0	fcc-FeH_x, FeH_2, dhcp-FeH_x
				68.2	dhcp-FeH_x, fcc-FeH_x	26	~1000	68.4	fcc-FeH_x, dhcp-FeH_x
8	Fe, liquid H_2	NaCl	300	49.0	dhcp-FeH_x, hcp-Fe	62	~1000	56.0	hcp-FeH_x
				44.9	hcp-FeH_x	5	~1000	53.3	hcp-FeH_x

TABLE S3. Experimental pressure-volume data of fcc FeH_x.

Run#	Pressure (GPa)	Pressure error (GPa)	Volume per Fe atom (Å^3)	Volume error (Å^3)	Pressure marker	Peaks used to determine *V*
1	65.10	1.96	10.994	0.012	Ruby	111, 200, 220
1	63.61	1.92	11.052	0.019	Ruby	111, 200, 220
1	55.21	1.66	11.142	0.024	Ruby	111, 200, 220
1	51.89	1.56	11.197	0.031	Ruby	111, 200, 220
1	45.35	1.37	11.275	0.029	Ruby	111, 200, 220
1	45.05	1.36	11.310	0.031	Ruby	111, 200, 220
1	41.46	1.25	11.399	0.035	Ruby	111, 200, 220
1	39.27	1.18	11.475	0.034	Ruby	111, 200, 220
1	36.47	1.10	11.536	0.034	Ruby	111, 200, 220
1	33.88	1.02	11.629	0.038	Ruby	111, 200, 220
1	30.37	0.91	11.753	0.048	Ruby	111, 200, 220
1	27.98	0.84	11.876	0.040	Ruby	111, 200, 220
1	24.60	0.74	12.120	0.038	Ruby	111, 200, 220
1	21.19	0.64	12.212	0.049	Ruby	111, 200, 220
1	18.31	0.55	12.381	0.039	Ruby	111, 200, 220
1	15.36	0.46	12.618	0.042	Ruby	111, 200, 220
2	64.24	-	10.993	0.014	KCl	111, 200, 220
2	64.22	-	10.899	0.016	KCl	111, 200, 220
2	67.15	-	10.781	0.022	KCl	111, 200, 220
2	74.25	-	10.533	0.025	KCl	111, 200, 220
2	76.96	-	10.396	0.023	KCl	111, 200, 220
2	78.60	-	10.396	0.023	KCl	111, 200, 220
2	79.68	-	10.356	0.024	KCl	111, 200, 220
2	81.71	-	10.292	0.026	KCl	111, 200, 220
2	105.33	-	9.976	0.011	KCl	111, 200, 220
2	107.06	-	9.916	0.012	KCl	111, 200, 220
2	111.90	-	9.842	0.014	KCl	111, 200, 220
2	109.88	-	9.815	0.016	KCl	111, 200, 220
2	115.53	-	9.759	0.014	KCl	111, 200, 220
2	116.80	-	9.697	0.013	KCl	111, 200, 220
3	43.58	-	11.313	0.025	KCl	111, 200, 220
3	56.79	-	11.019	0.025	KCl	111, 200, 220
3	67.24	-	10.743	0.156	KCl	111, 200, 220
3	68.98	-	10.601	0.040	KCl	111, 200, 220
3	76.25	-	10.420	0.023	KCl	111, 200, 220
3	87.51	-	10.321	0.048	KCl	111, 200, 220
3	90.13	-	10.256	0.055	KCl	111, 200, 220
3	89.93	-	10.177	0.069	KCl	111, 200, 220
3	100.93	-	10.049	0.001	KCl	111, 200, 220
3	93.39	-	10.146	0.038	KCl	111, 200, 220
3	85.90	-	10.290	0.058	KCl	111, 200, 220
3	86.30	-	10.340	0.015	KCl	111, 200, 220
3	84.32	-	10.316	0.053	KCl	111, 200, 220
3	83.44	-	10.331	0.031	KCl	111, 200, 220
3	84.03	-	10.344	0.031	KCl	111, 200, 220
3	86.39	-	10.301	0.084	KCl	111, 200, 220
3	77.33	-	10.403	0.098	KCl	111, 200, 220
4	126.26	0.09	9.470	0.004	NaCl	111, 200, 220
5	98.54	0.08	9.965	0.006	NaCl	111, 200, 220
5	99.09	0.05	9.942	0.006	NaCl	111, 200, 220
5	100.12	0.09	9.920	0.006	NaCl	111, 200, 220
5	100.98	0.14	9.906	0.006	NaCl	111, 200, 220
5	103.60	0.05	9.858	0.005	NaCl	111, 200, 220
5	113.65	0.16	9.708	0.003	NaCl	111, 200, 220
5	123.50	0.35	9.574	0.002	NaCl	111, 200, 220
5	128.36	0.86	9.510	0.001	NaCl	111, 200, 220
5	137.14	1.15	9.368	0.005	NaCl	111, 200, 220
6	91.34	0.49	10.027	0.029	NaCl	111, 200
6	99.28	0.22	9.949	0.006	NaCl	111, 200
6	104.77	0.37	9.815	0.003	NaCl	111, 200
6	75.09	0.39	10.348	-	NaCl	200
6	71.57	0.44	10.598	-	NaCl	200
6	66.19	0.28	10.699	-	NaCl	200
6	54.63	0.02	11.094	-	NaCl	200
6	25.59	0.11	11.923	0.016	NaCl	200, 220
7	68.41	0.17	10.543	0.021	NaCl	200, 220