Supporting Information

Pressure-Induced Crystal Structure and Spin-State Transitions in Magnetite (Fe_3O_4)

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1. Detailed lattice constants and atomic coordinate parameters for the nine typical samples. Table I for $Fd\bar{3}m$ phase. Table II and Table III for $Pbcm$ phase. Table IV and Table V for $Bbmm$ phase.

2. Orbital resolved density of states for the nine typical samples. Figure 1 for A-site Fe and Figure 2 for B-site Fe.

TABLE I: Lattice constant (Å) and atomic coordinate parameter of Fe_3O_4 (sample I, sample II, and sample III) with the space group $Fd\bar{3}m$.

Sample	I	II	III
a	8.4018	8.2333	8.0415
u	0.2546	0.2545	0.2544

TABLE II: Lattice constant (Å) of Fe_3O_4 (sample IV, sample V, and sample VI) with the space group *Pbcm*.

Sample	IV	V	VI
a	2.64872	2.59084	2.55332
b	9.31928	9.10468	9.00087
c	9.37144	9.20406	9.12054

TABLE III: Atomic coordinates (x,y,z) of Fe_3O_4 (sample IV, sample V, and sample VI) with the space group $Pbcm$.

Atom	Site	IV	V	VI
Fe1	4d	(0.74985,0.36270,0.25)	(0.74999,0.35843,0.25)	(0.74998,0.35643,0.25)
Fe2	8e	(0.24974,0.11603,0.07154)	(0.24999,0.11357,0.07109)	(0.24979,0.11244,0.07105)
O1	4c	(0.74946,0.25,0)	(0.74998,0.25,0)	(0.74986,0.25,0)
O2	4d	(0.24967,0.20465,0.25)	(0.25009,0.20016,0.25)	(0.24982,0.19803,0.25)
O3	8e	(0.24999,0.46650,0.11728)	(0.24990,0.46433,0.11889)	(0.25016,0.46335,0.11965)

TABLE IV: Lattice constant (Å) of Fe_3O_4 (sample VII, sample VIII, and sample IX) with the space group *Bbmm*.

Sample	VII	VIII	IX
a	8.98279	8.88086	8.84489
b	9.04893	8.89412	8.85431
c	2.54251	2.48289	2.46635

TABLE V: Atomic coordinates (x,y,z) of Fe_3O_4 (sample VII, sample VIII, and sample IX) with the space group $Bbmm$.

Atom	Site	VII	VIII	IX
Fe1	4c	(0.38484,0.25,0)	(0.38832,0.25,0)	(0.38970,0.25,0)
Fe2	8f	(0.13324,0.07290,0)	(0.13493,0.07291,0)	(0.13553,0.07279,0)
O1	4c	(0.04543,0.25,0)	(0.04731,0.25,0)	(0.04827,0.25,0)
O2	8f	(0.21872,0.61514,0)	(0.21718,0.61663,0)	(0.21656,0.61727,0)
O3	4a	(0.5,0,0)	(0.5,0,0)	(0.5,0,0)

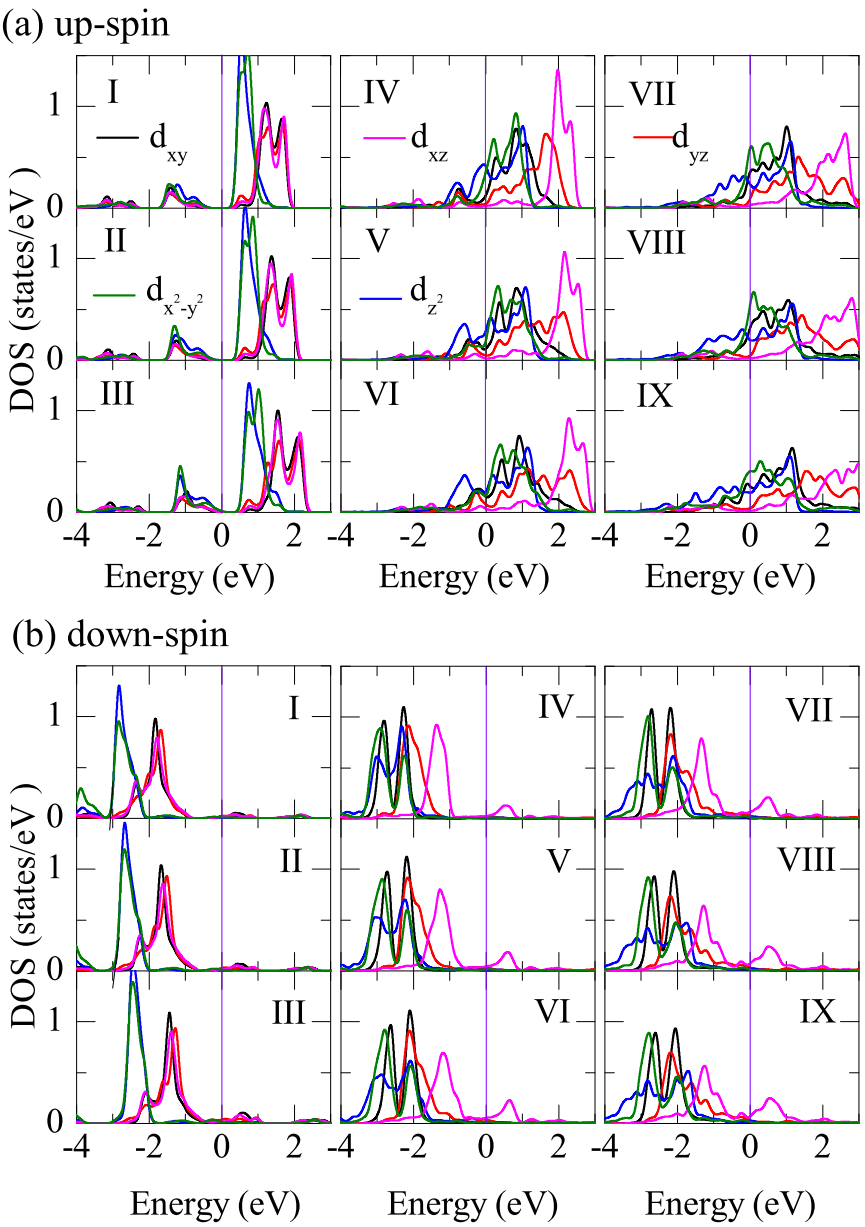

FIG. 1: 3*d*-orbital resolved local density of states of Fe ions at A-site for the nine typical samples. (a) Up-spin channel. (b) Down-spin channel. The vertical line indicates the Fermi level.

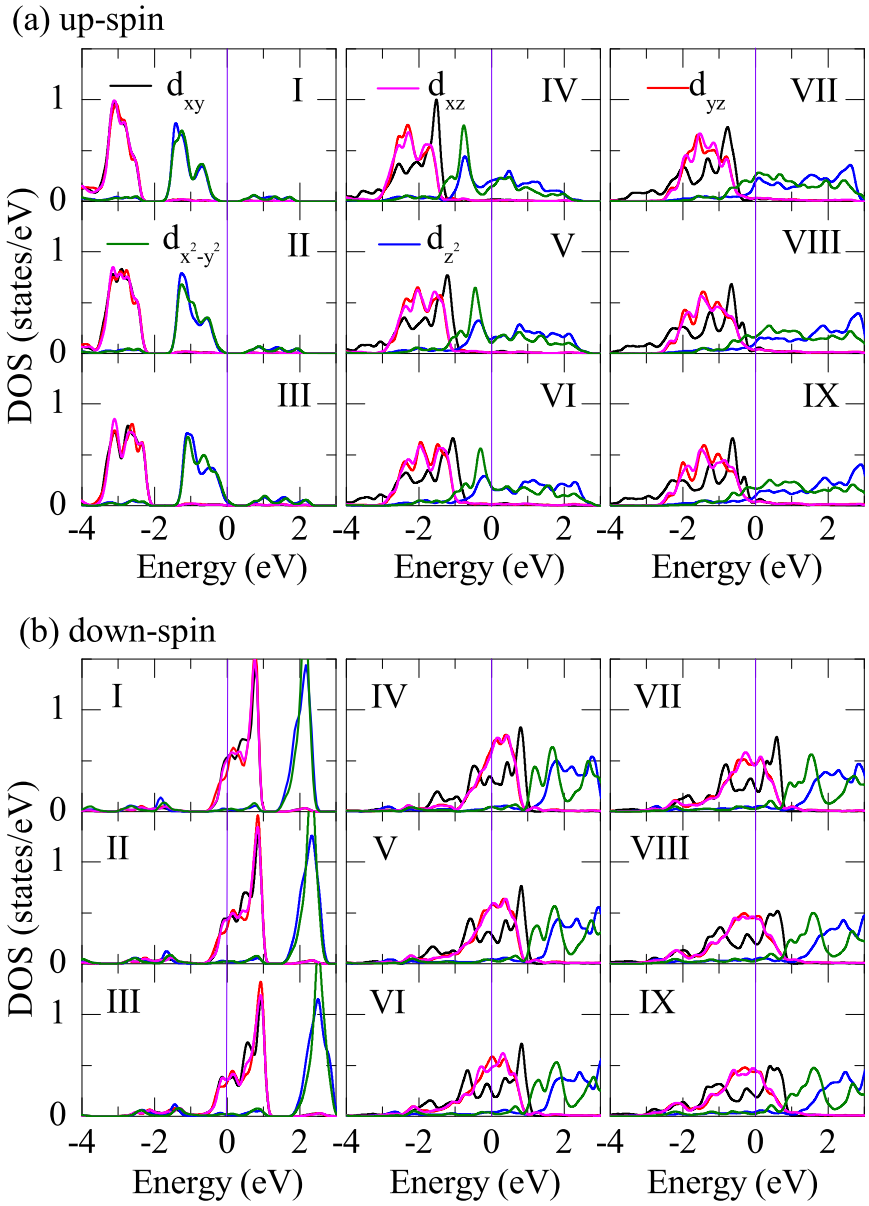

FIG. 2: 3*d*-orbital resolved local density of states of Fe ions at B-site for the nine typical samples. (a) Up-spin channel. (b) Down-spin channel. The vertical line indicates the Fermi level.