Supplementary

A Two-Stage Model of Verwey Transition in Fe_3O_4: First-Principles Studies

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<u>Section I.</u> Convergence test with respect to *k*-point mesh

As shown in the Fig. S1, the total energy of fully distorted Fe_3O_4 unit cell with *k*-point mesh of 2×2×2, 3×3×3, and 5×5×5 is tested. The total energies of Fe_3O_4 converge to -1557.7849619 eV and -1557.7849430 eV by using a 3×3×3 and 5×5×5 meshes, respectively. The energy difference between these two settings is only 1.89×10^{-5} eV/u.c. (~8.42×10^{-8} eV/atom). Thus, a 3×3×3 *k*-point mesh is sufficient for the Fe_3O_4 system.

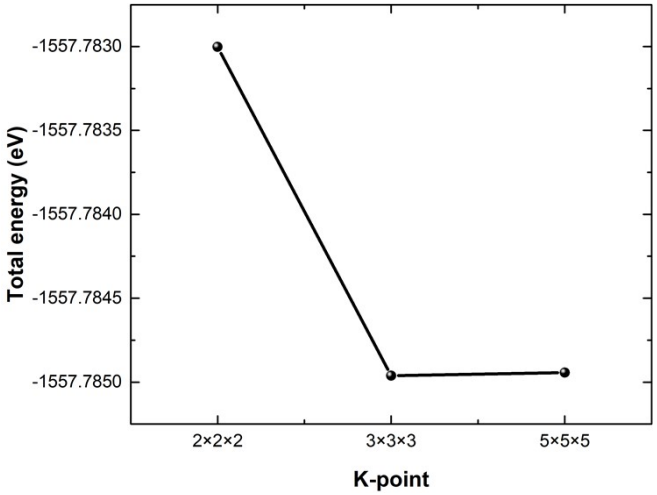

Fig. S1 The convergent total energy of fully distorted Fe_3O_4 with different *k*-point mesh.

Section II. Convergence test with respect to Hubbard *U*

As shown in Fig S2 to S4, the variations in total energy, band gap, charge, and magnetic moment for distortion levels of 10%, 20%, and 30% with Hubbard *U* parameter of 3, 3.5, 4, 4.5, 5, and 5.5 eV are calculated. Here, a uniform *J*=0.89 eV is introduced as mentioned in manuscript.

As shown in Fig. S2(a), the total energy with different *U* shows a similar trend as the distortion increases. For a given distortion level, the total energy increases with the increasing *U*, which is expected due to the enhancement of electron-electron repulsion introduced by *U*.

Figure S2(b) shows the dependence of band gap on the Hubbard *U*. The band gap increases with the increased *U*, which is in line with the previous results.[1] For *U*=3, the electron-electron interaction is too weak to open a band gap even the distortion reaches to 30%. For *U*=3.5 and 4 eV, the band gap gradually widens as the distortion increased. For *U*=4.5, 5 and 5.5 eV, the band gap increases with lattice distortion (e.g., at *d*=10%, 30%, and 100%), but exhibits a local minimum at *d*=20%.

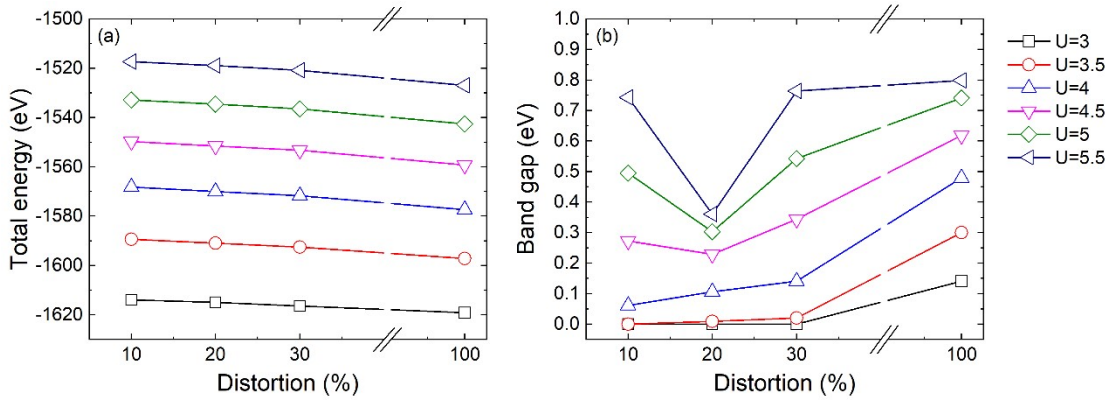

Fig. S2 The dependence of (a) total energy and (b) band gap on Hubbard *U*.

The charge ordering with different settings of U is examined. As shown in Fig. S3, clearly charge ordering can be observed for all cases except U=4 eV. However, an unexpected reversal of occurs between low and high U regimes. At U=3 and 3.5 eV, the Fe ions that exhibit divalent-like character at higher U (e.g., 4.5–5.5 eV) instead appear trivalent, and vice versa. The results obtained with smaller U show significant discrepancies compared to the experimental results as reported by Senn *et al.*[2] Consequently, we conclude that a small Hubbard U value is insufficient to reproduce the correct electronic structure of Fe_3O_4. In contrast, the results obtained with larger value, i.e., U=5 and 5.5 eV show similar trend compared to results with U=4.5 eV supporting the robustness of our findings. Although the charge separation gets larger with higher value of U, it is reasonable due to the increased electron-electron repulsion introduced by U as well.

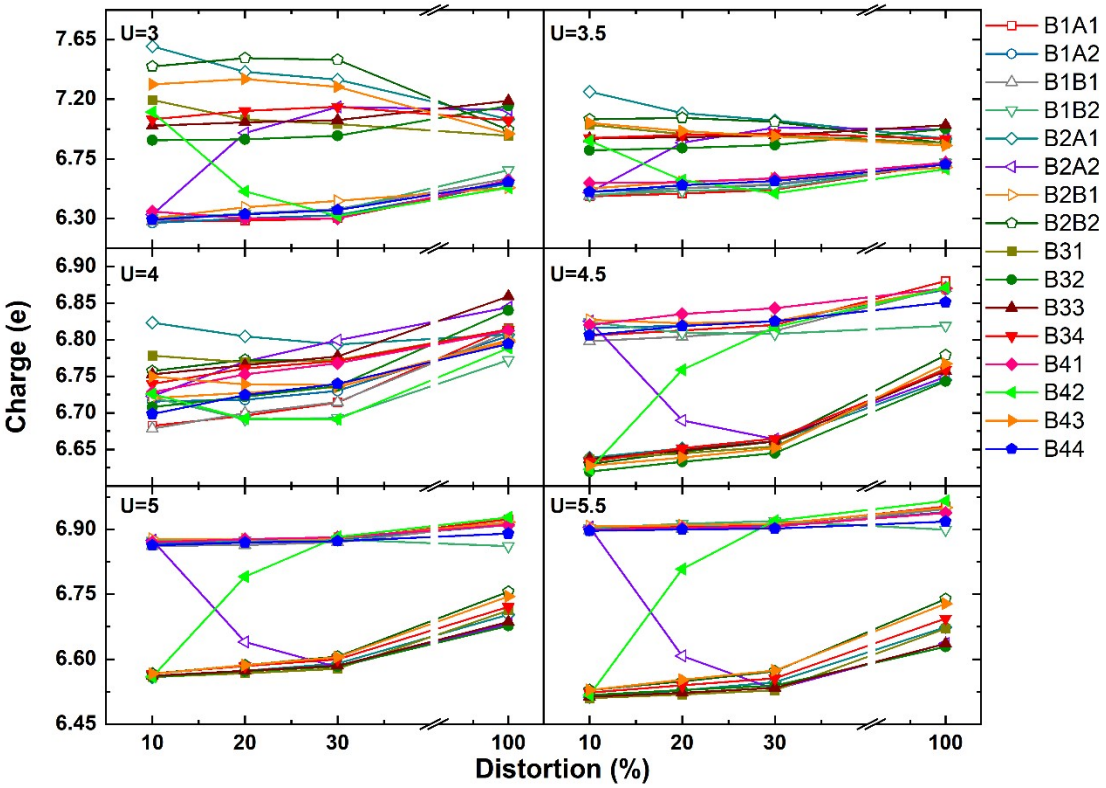

Fig. S3 The dependence of charge at Fe_B sites on distortion and Hubbard U.

Figure S4 shows the magnetic moment results with different settings of *U*. The magnetic moments show strongly dependence on the Hubbard *U* when the value is less than 4.5 eV. In contrast, the magnetic moments show similar dependence on the distortion when *U* is larger than 4.5 eV, which suppose that the utilize of GGA+*U* method with *U*=4.5 eV is reasonable to investigate the electronic structures of Fe_3O_4.

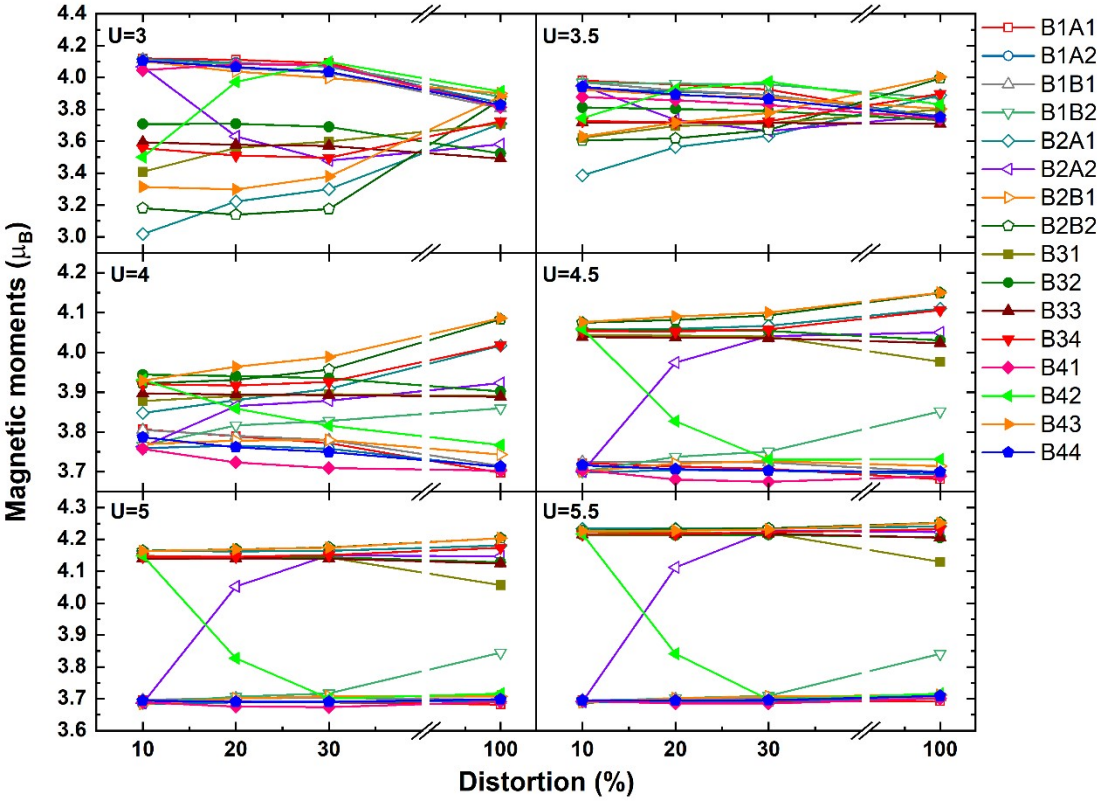

Fig. S4 The dependence of magnetic moments at Fe_B sites on distortion and Hubbard *U*.

<u>Section III.</u> The final geometries of the unit cells used in this work. The lattice constants are in VASP format.

Fe_3O_4 d=0%

Lattice constants:

8.3960000000000000	8.3960000000000000	0.0000000000000000
-8.3960000000000000	8.3960000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	16.7920000000000000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875000	0.875000	0.000000	O6B1	0.000000	0.000000	0.625000
O12	0.875000	0.375000	0.000000	O6B2	0.000000	0.500000	0.625000
O13	0.625000	0.875000	0.500000	O6B3	0.000000	0.000000	0.875000
O14	0.625000	0.375000	0.500000	O6B4	0.000000	0.500000	0.875000
O21	0.875000	0.625000	0.000000	FeA11	0.875000	0.750000	0.062500
O22	0.875000	0.125000	0.000000	FeA12	0.875000	0.250000	0.062500
O23	0.625000	0.625000	0.500000	FeA13	0.625000	0.750000	0.437500
O24	0.625000	0.125000	0.500000	FeA14	0.625000	0.250000	0.437500
O31	0.875000	0.875000	0.250000	FeA21	0.875000	0.500000	0.187500
O32	0.875000	0.375000	0.250000	FeA22	0.875000	0.000000	0.187500
O33	0.625000	0.875000	0.250000	FeA23	0.625000	0.500000	0.312500
O34	0.625000	0.375000	0.250000	FeA24	0.625000	0.000000	0.312500
O41	0.875000	0.625000	0.250000	FeB1A1	0.750000	0.000000	0.000000
O42	0.875000	0.125000	0.250000	FeB1A2	0.750000	0.500000	0.000000
O43	0.625000	0.625000	0.250000	FeB1B1	0.000000	0.500000	0.500000
O44	0.625000	0.125000	0.250000	FeB1B2	0.000000	0.000000	0.500000
O5A1	0.750000	0.750000	0.125000	FeB2A1	0.750000	0.750000	0.250000
O5A2	0.750000	0.250000	0.125000	FeB2A2	0.750000	0.250000	0.250000
O5A3	0.750000	0.750000	0.375000	FeB2B1	0.000000	0.750000	0.750000
O5A4	0.750000	0.250000	0.375000	FeB2B2	0.000000	0.250000	0.750000
O5B1	0.000000	0.750000	0.625000	FeB31	0.875000	0.875000	0.375000
O5B2	0.000000	0.250000	0.625000	FeB32	0.875000	0.375000	0.375000
O5B3	0.000000	0.750000	0.875000	FeB33	0.625000	0.875000	0.125000
O5B4	0.000000	0.250000	0.875000	FeB34	0.625000	0.375000	0.125000
O6A1	0.750000	0.500000	0.125000	FeB41	0.875000	0.625000	0.375000
O6A2	0.750000	0.000000	0.125000	FeB42	0.875000	0.125000	0.375000
O6A3	0.750000	0.500000	0.375000	FeB43	0.625000	0.625000	0.125000
O6A4	0.750000	0.000000	0.375000	FeB44	0.625000	0.125000	0.125000

Fe_3O_4 d=1%

Lattice constants:

8.3961065817100	8.3961065817100	0.0000000000000
-8.3958279109300	8.3958279109300	0.0000000000000
-0.0004892468392	-0.0004892468392	16.7918300731000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875008	0.875054	0.000001	O6B1	0.000110	-0.000023	0.624987
O12	0.875011	0.375057	-0.000016	O6B2	0.000028	0.499987	0.625011
O13	0.625019	0.875069	0.500050	O6B3	-0.000028	-0.000022	0.875013
O14	0.625006	0.375078	0.500058	O6B4	0.000007	0.499982	0.875024
O21	0.875014	0.624985	-0.000003	FeA11	0.875001	0.750013	0.062529
O22	0.875020	0.124988	0.000000	FeA12	0.875031	0.250020	0.062525
O23	0.624985	0.624983	0.500034	FeA13	0.624997	0.750028	0.437504
O24	0.625008	0.124997	0.500018	FeA14	0.625016	0.250040	0.437503
O31	0.875028	0.874947	0.250027	FeA21	0.874996	0.500048	0.187528
O32	0.874992	0.375010	0.250051	FeA22	0.875057	0.000007	0.187510
O33	0.625044	0.875019	0.249957	FeA23	0.625003	0.500016	0.312486
O34	0.624999	0.374948	0.249957	FeA24	0.625042	0.000050	0.312503
O41	0.875023	0.625125	0.250048	FeB1A1	0.750006	-0.000021	0.000023
O42	0.875030	0.125067	0.250018	FeB1A2	0.750012	0.499987	0.000011
O43	0.625044	0.625072	0.249968	FeB1B1	0.000019	0.500005	0.500017
O44	0.625021	0.125118	0.249993	FeB1B2	-0.000026	0.000008	0.499969
O5A1	0.749935	0.750005	0.125053	FeB2A1	0.749976	0.750064	0.250026
O5A2	0.749985	0.250064	0.125054	FeB2A2	0.750093	0.250022	0.250037
O5A3	0.750027	0.750052	0.374972	FeB2B1	0.000026	0.749937	0.750019
O5A4	0.750059	0.250074	0.374992	FeB2B2	0.000021	0.249959	0.750019
O5B1	0.000101	0.749979	0.625041	FeB31	0.875019	0.875045	0.375048
O5B2	0.000052	0.249949	0.625058	FeB32	0.875014	0.375125	0.375057
O5B3	-0.000051	0.749964	0.874972	FeB33	0.625016	0.875116	0.124968
O5B4	-0.000027	0.249944	0.874962	FeB34	0.625038	0.374996	0.124981
O6A1	0.749931	0.500027	0.125008	FeB41	0.875010	0.624998	0.375017
O6A2	0.750010	-0.000004	0.124998	FeB42	0.875004	0.125059	0.374994
O6A3	0.750024	0.500033	0.375015	FeB43	0.625007	0.625028	0.125008
O6A4	0.750096	0.000048	0.375017	FeB44	0.625029	0.125010	0.125015

Fe_3O_4 d=2%

Lattice constants:

8.3962131634200	8.3962131634200	0.0000000000000
-8.3956558218600	8.3956558218600	0.0000000000000
-0.0009784936784	-0.0009784936784	16.7916601462000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875016	0.875109	0.000003	O6B1	0.000220	-0.000046	0.624974
O12	0.875021	0.375114	-0.000033	O6B2	0.000056	0.499974	0.625022
O13	0.625038	0.875137	0.500100	O6B3	-0.000057	-0.000045	0.875026
O14	0.625011	0.375156	0.500116	O6B4	0.000014	0.499965	0.875048
O21	0.875027	0.624971	-0.000006	FeA11	0.875002	0.750027	0.062558
O22	0.875040	0.124976	0.000001	FeA12	0.875063	0.250041	0.062551
O23	0.624970	0.624966	0.500068	FeA13	0.624995	0.750055	0.437508
O24	0.625015	0.124995	0.500036	FeA14	0.625032	0.250080	0.437507
O31	0.875056	0.874893	0.250054	FeA21	0.874992	0.500095	0.187556
O32	0.874984	0.375020	0.250102	FeA22	0.875114	0.000015	0.187520
O33	0.625088	0.875038	0.249915	FeA23	0.625005	0.500032	0.312472
O34	0.624998	0.374896	0.249913	FeA24	0.625085	0.000100	0.312505
O41	0.875046	0.625250	0.250095	FeB1A1	0.750011	-0.000042	0.000045
O42	0.875060	0.125134	0.250036	FeB1A2	0.750023	0.499973	0.000022
O43	0.625088	0.625143	0.249936	FeB1B1	0.000037	0.500010	0.500034
O44	0.625042	0.125236	0.249985	FeB1B2	-0.000051	0.000015	0.499939
O5A1	0.749870	0.750010	0.125106	FeB2A1	0.749952	0.750128	0.250052
O5A2	0.749971	0.250129	0.125107	FeB2A2	0.750186	0.250044	0.250073
O5A3	0.750054	0.750104	0.374945	FeB2B1	0.000051	0.749874	0.750038
O5A4	0.750117	0.250147	0.374984	FeB2B2	0.000043	0.249918	0.750038
O5B1	0.000201	0.749959	0.625082	FeB31	0.875039	0.875089	0.375096
O5B2	0.000103	0.249898	0.625116	FeB32	0.875029	0.375249	0.375115
O5B3	-0.000103	0.749928	0.874943	FeB33	0.625033	0.875232	0.124936
O5B4	-0.000055	0.249888	0.874925	FeB34	0.625076	0.374992	0.124962
O6A1	0.749863	0.500055	0.125016	FeB41	0.875020	0.624996	0.375034
O6A2	0.750021	-0.000008	0.124995	FeB42	0.875009	0.125117	0.374987
O6A3	0.750048	0.500065	0.375030	FeB43	0.625013	0.625055	0.125017
O6A4	0.750192	0.000095	0.375034	FeB44	0.625058	0.125020	0.125030

Fe_3O_4 d=4%

Lattice constants:

8.3964263268400	8.3964263268400	0.0000000000000
-8.3953116437200	8.3953116437200	0.0000000000000
-0.0019569873568	-0.0019569873568	16.7913202924000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875032	0.875217	0.000006	O6B1	0.000440	-0.000092	0.624949
O12	0.875043	0.375229	-0.000066	O6B2	0.000111	0.499948	0.625043
O13	0.625076	0.875274	0.500200	O6B3	-0.000114	-0.000089	0.875052
O14	0.625022	0.375312	0.500232	O6B4	0.000027	0.499930	0.875096
O21	0.875054	0.624941	-0.000011	FeA11	0.875004	0.750053	0.062615
O22	0.875079	0.124951	0.000001	FeA12	0.875126	0.250082	0.062602
O23	0.624941	0.624932	0.500136	FeA13	0.624990	0.750110	0.437515
O24	0.625030	0.124990	0.500071	FeA14	0.625064	0.250159	0.437513
O31	0.875112	0.874786	0.250107	FeA21	0.874984	0.500191	0.187612
O32	0.874968	0.375041	0.250205	FeA22	0.875229	0.000030	0.187540
O33	0.625177	0.875076	0.249830	FeA23	0.625011	0.500065	0.312444
O34	0.624997	0.374792	0.249827	FeA24	0.625169	0.000201	0.312511
O41	0.875093	0.625500	0.250190	FeB1A1	0.750023	-0.000085	0.000091
O42	0.875120	0.125268	0.250072	FeB1A2	0.750046	0.499946	0.000045
O43	0.625175	0.625286	0.249872	FeB1B1	0.000075	0.500020	0.500068
O44	0.625083	0.125472	0.249970	FeB1B2	-0.000103	0.000030	0.499877
O5A1	0.749740	0.750020	0.125212	FeB2A1	0.749903	0.750256	0.250104
O5A2	0.749942	0.250258	0.125214	FeB2A2	0.750372	0.250088	0.250147
O5A3	0.750108	0.750207	0.374890	FeB2B1	0.000102	0.749749	0.750075
O5A4	0.750234	0.250295	0.374968	FeB2B2	0.000086	0.249835	0.750076
O5B1	0.000402	0.749917	0.625164	FeB31	0.875078	0.875178	0.375192
O5B2	0.000207	0.249796	0.625232	FeB32	0.875058	0.375499	0.375230
O5B3	-0.000206	0.749856	0.874887	FeB33	0.625065	0.875465	0.124871
O5B4	-0.000110	0.249776	0.874850	FeB34	0.625151	0.374985	0.124924
O6A1	0.749726	0.500110	0.125032	FeB41	0.875040	0.624993	0.375068
O6A2	0.750041	-0.000016	0.124990	FeB42	0.875017	0.125235	0.374975
O6A3	0.750096	0.500131	0.375061	FeB43	0.625026	0.625110	0.125034
O6A4	0.750385	0.000191	0.375068	FeB44	0.625115	0.125040	0.125061

Fe_3O_4 d=6%

Lattice constants:

8.3966394902600	8.3966394902600	0.0000000000000
-8.3949674655800	8.3949674655800	0.0000000000000
-0.0029354810352	-0.0029354810352	16.7909804386000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875049	0.875326	0.000008	O6B1	0.000659	-0.000137	0.624923
O12	0.875064	0.375343	-0.000098	O6B2	0.000167	0.499922	0.625065
O13	0.625115	0.875412	0.500300	O6B3	-0.000170	-0.000134	0.875077
O14	0.625034	0.375468	0.500347	O6B4	0.000041	0.499894	0.875144
O21	0.875082	0.624912	-0.000017	FeA11	0.875005	0.750080	0.062673
O22	0.875119	0.124927	0.000002	FeA12	0.875188	0.250122	0.062653
O23	0.624911	0.624898	0.500204	FeA13	0.624985	0.750166	0.437523
O24	0.625045	0.124984	0.500107	FeA14	0.625096	0.250239	0.437520
O31	0.875168	0.874680	0.250161	FeA21	0.874976	0.500286	0.187667
O32	0.874952	0.375061	0.250307	FeA22	0.875343	0.000044	0.187560
O33	0.625265	0.875115	0.249744	FeA23	0.625016	0.500097	0.312415
O34	0.624995	0.374688	0.249740	FeA24	0.625254	0.000301	0.312516
O41	0.875139	0.625749	0.250286	FeB1A1	0.750034	-0.000127	0.000136
O42	0.875181	0.125401	0.250108	FeB1A2	0.750070	0.499919	0.000067
O43	0.625263	0.625430	0.249809	FeB1B1	0.000112	0.500030	0.500102
O44	0.625125	0.125708	0.249955	FeB1B2	-0.000154	0.000046	0.499816
O5A1	0.749610	0.750030	0.125318	FeB2A1	0.749855	0.750383	0.250156
O5A2	0.749912	0.250386	0.125321	FeB2A2	0.750557	0.250132	0.250220
O5A3	0.750163	0.750311	0.374834	FeB2B1	0.000153	0.749623	0.750113
O5A4	0.750352	0.250442	0.374952	FeB2B2	0.000128	0.249753	0.750115
O5B1	0.000604	0.749876	0.625245	FeB31	0.875116	0.875267	0.375288
O5B2	0.000310	0.249694	0.625348	FeB32	0.875086	0.375748	0.375345
O5B3	-0.000309	0.749785	0.874830	FeB33	0.625098	0.875697	0.124807
O5B4	-0.000164	0.249663	0.874774	FeB34	0.625227	0.374977	0.124887
O6A1	0.749589	0.500165	0.125049	FeB41	0.875059	0.624989	0.375102
O6A2	0.750062	-0.000024	0.124986	FeB42	0.875026	0.125352	0.374962
O6A3	0.750143	0.500196	0.375091	FeB43	0.625040	0.625166	0.125050
O6A4	0.750577	0.000286	0.375102	FeB44	0.625173	0.125061	0.125091

Fe_3O_4 d=8%

Lattice constants:

8.3968526536800	8.3968526536800	0.0000000000000
-8.3946232874400	8.3946232874400	0.0000000000000
-0.0039139747136	-0.0039139747136	16.7906405848000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875065	0.875434	0.000011	O6B1	0.000879	-0.000183	0.624898
O12	0.875086	0.375458	-0.000131	O6B2	0.000222	0.499896	0.625086
O13	0.625153	0.875549	0.500400	O6B3	-0.000227	-0.000178	0.875103
O14	0.625045	0.375624	0.500463	O6B4	0.000054	0.499859	0.875192
O21	0.875109	0.624882	-0.000022	FeA11	0.875007	0.750106	0.062730
O22	0.875158	0.124902	0.000002	FeA12	0.875251	0.250163	0.062704
O23	0.624882	0.624864	0.500272	FeA13	0.624980	0.750221	0.437530
O24	0.625060	0.124979	0.500142	FeA14	0.625128	0.250318	0.437526
O31	0.875224	0.874573	0.250214	FeA21	0.874969	0.500382	0.187723
O32	0.874936	0.375082	0.250410	FeA22	0.875458	0.000059	0.187580
O33	0.625354	0.875153	0.249659	FeA23	0.625021	0.500130	0.312387
O34	0.624994	0.374584	0.249654	FeA24	0.625338	0.000402	0.312522
O41	0.875186	0.625999	0.250381	FeB1A1	0.750046	-0.000170	0.000182
O42	0.875241	0.125535	0.250144	FeB1A2	0.750093	0.499892	0.000089
O43	0.625350	0.625573	0.249745	FeB1B1	0.000150	0.500040	0.500136
O44	0.625166	0.125944	0.249940	FeB1B2	-0.000206	0.000061	0.499754
O5A1	0.749480	0.750040	0.125424	FeB2A1	0.749806	0.750511	0.250208
O5A2	0.749883	0.250515	0.125428	FeB2A2	0.750743	0.250176	0.250294
O5A3	0.750217	0.750414	0.374779	FeB2B1	0.000204	0.749498	0.750150
O5A4	0.750469	0.250590	0.374936	FeB2B2	0.000171	0.249670	0.750153
O5B1	0.000805	0.749834	0.625327	FeB31	0.875155	0.875356	0.375384
O5B2	0.000414	0.249592	0.625464	FeB32	0.875115	0.375998	0.375460
O5B3	-0.000412	0.749713	0.874774	FeB33	0.625130	0.875930	0.124742
O5B4	-0.000219	0.249551	0.874699	FeB34	0.625302	0.374970	0.124849
O6A1	0.749452	0.500220	0.125065	FeB41	0.875079	0.624986	0.375136
O6A2	0.750082	-0.000032	0.124981	FeB42	0.875034	0.125470	0.374949
O6A3	0.750191	0.500262	0.375122	FeB43	0.625053	0.625221	0.125067
O6A4	0.750770	0.000382	0.375136	FeB44	0.625230	0.125081	0.125121

Fe_3O_4 d=10%

Lattice constants:

8.3970658171000	8.3970658171000	0.0000000000000
-8.3942791093000	8.3942791093000	0.0000000000000
-0.0048924683920	-0.0048924683920	16.7903007310000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875081	0.875543	0.000014	O6B1	0.001099	-0.000229	0.624872
O12	0.875107	0.375572	-0.000164	O6B2	0.000278	0.499870	0.625108
O13	0.625191	0.875686	0.500500	O6B3	-0.000284	-0.000223	0.875129
O14	0.625056	0.375780	0.500579	O6B4	0.000068	0.499824	0.875240
O21	0.875136	0.624853	-0.000028	FeA11	0.875009	0.750133	0.062788
O22	0.875198	0.124878	0.000003	FeA12	0.875314	0.250204	0.062755
O23	0.624852	0.624830	0.500340	FeA13	0.624975	0.750276	0.437538
O24	0.625075	0.124974	0.500178	FeA14	0.62516	0.250398	0.437533
O31	0.87528	0.874466	0.250268	FeA21	0.874961	0.500477	0.187779
O32	0.87492	0.375102	0.250512	FeA22	0.875572	0.000074	0.187601
O33	0.625442	0.875191	0.249574	FeA23	0.625026	0.500162	0.312359
O34	0.624992	0.374480	0.249567	FeA24	0.625423	0.000502	0.312528
O41	0.875232	0.626249	0.250476	FeB1A1	0.750057	-0.000212	0.000227
O42	0.875301	0.125669	0.250180	FeB1A2	0.750116	0.499865	0.000111
O43	0.625438	0.625716	0.249681	FeB1B1	0.000187	0.500050	0.500170
O44	0.625208	0.126180	0.249925	FeB1B2	-0.000257	0.000076	0.499693
O5A1	0.74935	0.750050	0.125530	FeB2A1	0.749758	0.750639	0.250260
O5A2	0.749854	0.250644	0.125535	FeB2A2	0.750929	0.250220	0.250367
O5A3	0.750271	0.750518	0.374724	FeB2B1	0.000255	0.749372	0.750188
O5A4	0.750586	0.250737	0.374920	FeB2B2	0.000214	0.249588	0.750191
O5B1	0.001006	0.749793	0.625409	FeB31	0.875194	0.875445	0.375480
O5B2	0.000517	0.249490	0.625580	FeB32	0.875144	0.376247	0.375575
O5B3	-0.000515	0.749641	0.874717	FeB33	0.625163	0.876162	0.124678
O5B4	-0.000274	0.249439	0.874624	FeB34	0.625378	0.374962	0.124811
O6A1	0.749315	0.500275	0.125081	FeB41	0.875099	0.624982	0.375171
O6A2	0.750103	-0.000040	0.124976	FeB42	0.875043	0.125587	0.374937
O6A3	0.750239	0.500327	0.375152	FeB43	0.625066	0.625276	0.125084
O6A4	0.750962	0.000477	0.375170	FeB44	0.625288	0.125101	0.125152

Fe_3O_4 d=20%

Lattice constants:

8.3981316342000	8.3981316342000	0.0000000000000
-8.3925582186000	8.3925582186000	0.0000000000000
-0.0097849367840	-0.0097849367840	16.7886014620000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875162	0.876086	0.000028	O6B1	0.002198	-0.000458	0.624744
O12	0.875214	0.376144	-0.000328	O6B2	0.000556	0.499740	0.625216
O13	0.625382	0.876372	0.501000	O6B3	-0.000568	-0.000446	0.875258
O14	0.625112	0.376560	0.501158	O6B4	0.000136	0.499648	0.875480
O21	0.875272	0.624706	-0.000056	FeA11	0.875018	0.750266	0.063075
O22	0.875396	0.124756	0.000006	FeA12	0.875628	0.250408	0.063009
O23	0.624704	0.624660	0.500680	FeA13	0.62495	0.750552	0.437575
O24	0.62515	0.124948	0.500356	FeA14	0.62532	0.250796	0.437566
O31	0.87556	0.873932	0.250536	FeA21	0.874921	0.500954	0.188058
O32	0.87484	0.375204	0.251024	FeA22	0.876144	0.000148	0.187701
O33	0.625884	0.875382	0.249148	FeA23	0.625053	0.500324	0.312218
O34	0.624984	0.373960	0.249134	FeA24	0.625846	0.001005	0.312555
O41	0.875464	0.627498	0.250952	FeB1A1	0.750114	-0.000424	0.000455
O42	0.875602	0.126338	0.250360	FeB1A2	0.750232	0.499730	0.000223
O43	0.625876	0.626432	0.249362	FeB1B1	0.000374	0.500100	0.500340
O44	0.625416	0.127360	0.249850	FeB1B2	-0.000514	0.000152	0.499386
O5A1	0.7487	0.750100	0.126060	FeB2A1	0.749516	0.751278	0.250520
O5A2	0.749708	0.251288	0.126070	FeB2A2	0.751858	0.250439	0.250735
O5A3	0.750542	0.751036	0.374448	FeB2B1	0.00051	0.748744	0.750375
O5A4	0.751172	0.251474	0.374840	FeB2B2	0.000428	0.249176	0.750382
O5B1	0.002012	0.749586	0.625818	FeB31	0.875388	0.875890	0.375961
O5B2	0.001034	0.248980	0.626160	FeB32	0.875288	0.377495	0.376150
O5B3	-0.00103	0.749282	0.874434	FeB33	0.625326	0.877325	0.124355
O5B4	-0.000548	0.248878	0.874248	FeB34	0.625756	0.374924	0.124622
O6A1	0.74863	0.500550	0.125162	FeB41	0.875198	0.624964	0.375341
O6A2	0.750206	-0.000080	0.124952	FeB42	0.875086	0.126174	0.374873
O6A3	0.750478	0.500654	0.375304	FeB43	0.625132	0.625552	0.125168
O6A4	0.751924	0.000954	0.375340	FeB44	0.625576	0.125202	0.125303

Fe_3O_4 d=30%

Lattice constants:

8.3991974513000	8.3991974513000	0.0000000000000
-8.3908373279000	8.3908373279000	0.0000000000000
-0.0146774051760	-0.0146774051760	16.7869021930000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875243	0.876629	0.000042	O6B1	0.003297	-0.000687	0.624616
O12	0.875321	0.376716	-0.000492	O6B2	0.000834	0.499610	0.625324
O13	0.625573	0.877058	0.501500	O6B3	-0.000852	-0.000669	0.875387
O14	0.625168	0.377340	0.501737	O6B4	0.000204	0.499472	0.875720
O21	0.875408	0.624559	-0.000084	FeA11	0.875027	0.750399	0.063363
O22	0.875594	0.124634	0.000009	FeA12	0.875942	0.250612	0.063264
O23	0.624556	0.624490	0.501020	FeA13	0.624925	0.750828	0.437613
O24	0.625225	0.124922	0.500534	FeA14	0.62548	0.251194	0.437599
O31	0.87584	0.873398	0.250804	FeA21	0.874882	0.501431	0.188337
O32	0.87476	0.375306	0.251536	FeA22	0.876717	0.000222	0.187802
O33	0.626326	0.875573	0.248722	FeA23	0.625079	0.500486	0.312077
O34	0.624976	0.373440	0.248701	FeA24	0.626269	0.001507	0.312582
O41	0.875696	0.628747	0.251428	FeB1A1	0.750171	-0.000636	0.000682
O42	0.875903	0.127007	0.250540	FeB1A2	0.750348	0.499595	0.000334
O43	0.626314	0.627148	0.249043	FeB1B1	0.000561	0.500150	0.500510
O44	0.625624	0.128540	0.249775	FeB1B2	-0.000771	0.000228	0.499079
O5A1	0.74805	0.750150	0.126590	FeB2A1	0.749274	0.751917	0.250781
O5A2	0.749562	0.251932	0.126605	FeB2A2	0.752787	0.250659	0.251102
O5A3	0.750813	0.751554	0.374172	FeB2B1	0.000765	0.748116	0.750563
O5A4	0.751758	0.252211	0.374760	FeB2B2	0.000642	0.248764	0.750573
O5B1	0.003018	0.749379	0.626227	FeB31	0.875582	0.876335	0.376441
O5B2	0.001551	0.248470	0.626740	FeB32	0.875432	0.378742	0.376725
O5B3	-0.001545	0.748923	0.874151	FeB33	0.625489	0.878487	0.124033
O5B4	-0.000822	0.248317	0.873872	FeB34	0.626134	0.374886	0.124434
O6A1	0.747945	0.500825	0.125243	FeB41	0.875297	0.624946	0.375512
O6A2	0.750309	-0.000120	0.124928	FeB42	0.875129	0.126761	0.374810
O6A3	0.750717	0.500981	0.375456	FeB43	0.625198	0.625828	0.125252
O6A4	0.752886	0.001431	0.375510	FeB44	0.625864	0.125303	0.125455

Fe_3O_4 d=40%

Lattice constants:

8.4002632684000	8.4002632684000	0.0000000000000
-8.3891164372000	8.3891164372000	0.0000000000000
-0.0195698735680	-0.0195698735680	16.7852029240000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875324	0.877172	0.000056	O6B1	0.004396	-0.000916	0.624488
O12	0.875428	0.377288	-0.000656	O6B2	0.001112	0.499480	0.625432
O13	0.625764	0.877744	0.502000	O6B3	-0.001136	-0.000892	0.875516
O14	0.625224	0.378120	0.502316	O6B4	0.000272	0.499296	0.875960
O21	0.875544	0.624412	-0.000112	FeA11	0.875036	0.750532	0.063651
O22	0.875792	0.124512	0.000012	FeA12	0.876256	0.250816	0.063518
O23	0.624408	0.624320	0.501360	FeA13	0.624900	0.751104	0.437651
O24	0.625300	0.124896	0.500712	FeA14	0.625640	0.251592	0.437632
O31	0.876120	0.872864	0.251072	FeA21	0.874843	0.501908	0.188616
O32	0.874680	0.375408	0.252048	FeA22	0.877289	0.000296	0.187902
O33	0.626768	0.875764	0.248296	FeA23	0.625105	0.500648	0.311936
O34	0.624968	0.372920	0.248268	FeA24	0.626692	0.002010	0.312610
O41	0.875928	0.629996	0.251904	FeB1A1	0.750228	-0.000848	0.000909
O42	0.876204	0.127676	0.250720	FeB1A2	0.750464	0.499460	0.000446
O43	0.626752	0.627864	0.248724	FeB1B1	0.000748	0.500200	0.500680
O44	0.625832	0.129720	0.249700	FeB1B2	-0.001028	0.000304	0.498772
O5A1	0.747400	0.750200	0.127120	FeB2A1	0.749032	0.752556	0.251041
O5A2	0.749416	0.252576	0.127140	FeB2A2	0.753716	0.250879	0.251469
O5A3	0.751084	0.752072	0.373896	FeB2B1	0.001020	0.747488	0.750751
O5A4	0.752344	0.252948	0.374680	FeB2B2	0.000856	0.248352	0.750764
O5B1	0.004024	0.749172	0.626636	FeB31	0.875776	0.876780	0.376922
O5B2	0.002068	0.247960	0.627320	FeB32	0.875576	0.379989	0.377300
O5B3	-0.002060	0.748564	0.873868	FeB33	0.625652	0.879650	0.123710
O5B4	-0.001096	0.247756	0.873496	FeB34	0.626512	0.374848	0.124245
O6A1	0.747260	0.501100	0.125324	FeB41	0.875396	0.624928	0.375682
O6A2	0.750412	-0.000160	0.124904	FeB42	0.875172	0.127348	0.374746
O6A3	0.750956	0.501308	0.375608	FeB43	0.625264	0.626104	0.125336
O6A4	0.753848	0.001908	0.375680	FeB44	0.626152	0.125404	0.125607

Fe_3O_4 d=50%

Lattice constants:

8.4013290855000	8.4013290855000	0.0000000000000
-8.3873955465000	8.3873955465000	0.0000000000000
-0.0244623419600	-0.0244623419600	16.7835036550000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875405	0.877715	0.000070	O6B1	0.005495	-0.001145	0.624360
O12	0.875535	0.377860	-0.000820	O6B2	0.001390	0.499350	0.625540
O13	0.625955	0.878430	0.502500	O6B3	-0.001420	-0.001115	0.875645
O14	0.625280	0.378900	0.502895	O6B4	0.000340	0.499120	0.876200
O21	0.875680	0.624265	-0.000140	FeA11	0.875045	0.750665	0.063939
O22	0.875990	0.124390	0.000015	FeA12	0.876570	0.251020	0.063773
O23	0.624260	0.624150	0.501700	FeA13	0.624875	0.751380	0.437689
O24	0.625375	0.124870	0.500890	FeA14	0.625800	0.251990	0.437665
O31	0.876400	0.872330	0.251340	FeA21	0.874804	0.502385	0.188895
O32	0.874600	0.375510	0.252560	FeA22	0.877861	0.000370	0.188003
O33	0.627210	0.875955	0.247870	FeA23	0.625131	0.500810	0.311795
O34	0.624960	0.372400	0.247835	FeA24	0.627115	0.002512	0.312638
O41	0.876160	0.631245	0.252380	FeB1A1	0.750285	-0.001060	0.001136
O42	0.876505	0.128345	0.250900	FeB1A2	0.750580	0.499325	0.000557
O43	0.627190	0.628580	0.248405	FeB1B1	0.000935	0.500250	0.500850
O44	0.626040	0.130900	0.249625	FeB1B2	-0.001285	0.000380	0.498466
O5A1	0.746750	0.750250	0.127650	FeB2A1	0.748790	0.753196	0.251301
O5A2	0.749270	0.253220	0.127675	FeB2A2	0.754645	0.251099	0.251837
O5A3	0.751355	0.752590	0.373620	FeB2B1	0.001275	0.746860	0.750938
O5A4	0.752930	0.253685	0.374600	FeB2B2	0.001070	0.247940	0.750955
O5B1	0.005030	0.748965	0.627045	FeB31	0.875970	0.877225	0.377402
O5B2	0.002585	0.247450	0.627900	FeB32	0.875720	0.381236	0.377875
O5B3	-0.002575	0.748205	0.873585	FeB33	0.625815	0.880812	0.123388
O5B4	-0.001370	0.247195	0.873120	FeB34	0.626890	0.374810	0.124056
O6A1	0.746575	0.501375	0.125405	FeB41	0.875495	0.624910	0.375853
O6A2	0.750515	-0.000200	0.124880	FeB42	0.875215	0.127935	0.374683
O6A3	0.751195	0.501635	0.375760	FeB43	0.625330	0.626380	0.125420
O6A4	0.754810	0.002385	0.375850	FeB44	0.626440	0.125505	0.125758

Fe_3O_4 d=60%

Lattice constants:

8.4023949026000	8.4023949026000	0.0000000000000
-8.3856746558000	8.3856746558000	0.0000000000000
-0.0293548103520	-0.0293548103520	16.7818043860000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875486	0.878258	0.000084	O6B1	0.006594	-0.001374	0.624232
O12	0.875642	0.378432	-0.000984	O6B2	0.001668	0.499220	0.625648
O13	0.626146	0.879116	0.503000	O6B3	-0.001704	-0.001338	0.875774
O14	0.625336	0.379680	0.503474	O6B4	0.000408	0.498944	0.876440
O21	0.875816	0.624118	-0.000168	FeA11	0.875054	0.750798	0.064226
O22	0.876188	0.124268	0.000018	FeA12	0.876884	0.251224	0.064028
O23	0.624112	0.623980	0.502040	FeA13	0.624850	0.751656	0.437726
O24	0.625450	0.124844	0.501068	FeA14	0.625960	0.252388	0.437698
O31	0.876680	0.871796	0.251608	FeA21	0.874764	0.502862	0.189174
O32	0.874520	0.375612	0.253072	FeA22	0.878433	0.000444	0.188104
O33	0.627652	0.876146	0.247444	FeA23	0.625158	0.500972	0.311654
O34	0.624952	0.371880	0.247402	FeA24	0.627537	0.003014	0.312665
O41	0.876392	0.632494	0.252856	FeB1A1	0.750342	-0.001272	0.001364
O42	0.876806	0.129014	0.251080	FeB1A2	0.750696	0.499190	0.000668
O43	0.627628	0.629296	0.248086	FeB1B1	0.001122	0.500300	0.501020
O44	0.626248	0.132080	0.249550	FeB1B2	-0.001542	0.000456	0.498159
O5A1	0.746100	0.750300	0.128180	FeB2A1	0.748548	0.753835	0.251561
O5A2	0.749124	0.253864	0.128210	FeB2A2	0.755574	0.251318	0.252204
O5A3	0.751626	0.753108	0.373344	FeB2B1	0.001530	0.746232	0.751126
O5A4	0.753516	0.254422	0.374520	FeB2B2	0.001284	0.247528	0.751146
O5B1	0.006036	0.748758	0.627454	FeB31	0.876164	0.877670	0.377883
O5B2	0.003102	0.246940	0.628480	FeB32	0.875864	0.382484	0.378449
O5B3	-0.003090	0.747846	0.873302	FeB33	0.625978	0.881974	0.123066
O5B4	-0.001644	0.246634	0.872744	FeB34	0.627268	0.374773	0.123867
O6A1	0.745890	0.501650	0.125486	FeB41	0.875594	0.624892	0.376024
O6A2	0.750618	-0.000240	0.124856	FeB42	0.875258	0.128522	0.374619
O6A3	0.751434	0.501962	0.375912	FeB43	0.625396	0.626656	0.125504
O6A4	0.755772	0.002862	0.376020	FeB44	0.626728	0.125606	0.125910

Fe_3O_4 d=70%

Lattice constants:

8.4034607197000	8.4034607197000	0.0000000000000
-8.3839537651000	8.3839537651000	0.0000000000000
-0.0342472787440	-0.0342472787440	16.7801051170000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875567	0.878801	0.000098	O6B1	0.007693	-0.001603	0.624104
O12	0.875749	0.379004	-0.001148	O6B2	0.001946	0.499090	0.625756
O13	0.626337	0.879802	0.503500	O6B3	-0.001988	-0.001561	0.875903
O14	0.625392	0.380460	0.504053	O6B4	0.000476	0.498768	0.876680
O21	0.875952	0.623971	-0.000196	FeA11	0.875063	0.750931	0.064514
O22	0.876386	0.124146	0.000021	FeA12	0.877198	0.251428	0.064282
O23	0.623964	0.623810	0.502380	FeA13	0.624825	0.751932	0.437764
O24	0.625525	0.124818	0.501246	FeA14	0.626120	0.252786	0.437731
O31	0.876960	0.871262	0.251876	FeA21	0.874725	0.503339	0.189453
O32	0.874440	0.375714	0.253584	FeA22	0.879005	0.000518	0.188204
O33	0.628094	0.876337	0.247018	FeA23	0.625184	0.501134	0.311513
O34	0.624944	0.371360	0.246969	FeA24	0.627960	0.003517	0.312693
O41	0.876624	0.633743	0.253332	FeB1A1	0.750399	-0.001484	0.001591
O42	0.877107	0.129683	0.251260	FeB1A2	0.750812	0.499055	0.000780
O43	0.628066	0.630012	0.247767	FeB1B1	0.001309	0.500350	0.501190
O44	0.626456	0.133260	0.249475	FeB1B2	-0.001799	0.000532	0.497852
O5A1	0.745450	0.750350	0.128710	FeB2A1	0.748306	0.754474	0.251821
O5A2	0.748978	0.254508	0.128745	FeB2A2	0.756503	0.251538	0.252571
O5A3	0.751897	0.753626	0.373068	FeB2B1	0.001785	0.745604	0.751314
O5A4	0.754102	0.255159	0.374440	FeB2B2	0.001498	0.247116	0.751337
O5B1	0.007042	0.748551	0.627863	FeB31	0.876358	0.878115	0.378364
O5B2	0.003619	0.246430	0.629060	FeB32	0.876008	0.383731	0.379024
O5B3	-0.003605	0.747487	0.873019	FeB33	0.626141	0.883137	0.122743
O5B4	-0.001918	0.246073	0.872368	FeB34	0.627646	0.374735	0.123678
O6A1	0.745205	0.501925	0.125567	FeB41	0.875693	0.624874	0.376194
O6A2	0.750721	-0.000280	0.124832	FeB42	0.875301	0.129109	0.374555
O6A3	0.751673	0.502289	0.376064	FeB43	0.625462	0.626932	0.125588
O6A4	0.756734	0.003339	0.376190	FeB44	0.627016	0.125707	0.126062

Fe_3O_4 d=80%

Lattice constants:

8.4045265368000	8.4045265368000	0.0000000000000
-8.3822328744000	8.3822328744000	0.0000000000000
-0.0391397471360	-0.0391397471360	16.7784058480000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875648	0.879344	0.000112	O6B1	0.008792	-0.001832	0.623976
O12	0.875856	0.379576	-0.001312	O6B2	0.002224	0.498960	0.625864
O13	0.626528	0.880488	0.504000	O6B3	-0.002272	-0.001784	0.876032
O14	0.625448	0.381240	0.504632	O6B4	0.000544	0.498592	0.876920
O21	0.876088	0.623824	-0.000224	FeA11	0.875072	0.751064	0.064802
O22	0.876584	0.124024	0.000024	FeA12	0.877512	0.251632	0.064537
O23	0.623816	0.623640	0.502720	FeA13	0.624800	0.752208	0.437802
O24	0.625600	0.124792	0.501424	FeA14	0.626280	0.253184	0.437764
O31	0.877240	0.870728	0.252144	FeA21	0.874686	0.503816	0.189732
O32	0.874360	0.375816	0.254096	FeA22	0.879578	0.000592	0.188305
O33	0.628536	0.876528	0.246592	FeA23	0.625210	0.501296	0.311372
O34	0.624936	0.370840	0.246536	FeA24	0.628383	0.004019	0.312720
O41	0.876856	0.634992	0.253808	FeB1A1	0.750456	-0.001696	0.001818
O42	0.877408	0.130352	0.251440	FeB1A2	0.750928	0.498920	0.000891
O43	0.628504	0.630728	0.247448	FeB1B1	0.001496	0.500400	0.501360
O44	0.626664	0.134440	0.249400	FeB1B2	-0.002056	0.000608	0.497545
O5A1	0.744800	0.750400	0.129240	FeB2A1	0.748064	0.755113	0.252082
O5A2	0.748832	0.255152	0.129280	FeB2A2	0.757432	0.251758	0.252938
O5A3	0.752168	0.754144	0.372792	FeB2B1	0.002040	0.744976	0.751502
O5A4	0.754688	0.255896	0.374360	FeB2B2	0.001712	0.246704	0.751528
O5B1	0.008048	0.748344	0.628272	FeB31	0.876552	0.878560	0.378844
O5B2	0.004136	0.245920	0.629640	FeB32	0.876152	0.384978	0.379599
O5B3	-0.004120	0.747128	0.872736	FeB33	0.626304	0.884299	0.122421
O5B4	-0.002192	0.245512	0.871992	FeB34	0.628024	0.374697	0.123490
O6A1	0.744520	0.502200	0.125648	FeB41	0.875792	0.624856	0.376365
O6A2	0.750824	-0.000320	0.124808	FeB42	0.875344	0.129696	0.374492
O6A3	0.751912	0.502616	0.376216	FeB43	0.625528	0.627208	0.125672
O6A4	0.757696	0.003816	0.376360	FeB44	0.627304	0.125808	0.126214

Fe_3O_4 d=90%

Lattice constants:

8.4055923539000	8.4055923539000	0.0000000000000
-8.3805119837000	8.3805119837000	0.0000000000000
-0.0440322155280	-0.0440322155280	16.7767065790000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875729	0.879887	0.000126	O6B1	0.009891	-0.002061	0.623848
O12	0.875963	0.380148	-0.001476	O6B2	0.002502	0.498830	0.625972
O13	0.626719	0.881174	0.504500	O6B3	-0.002556	-0.002007	0.876161
O14	0.625504	0.382020	0.505211	O6B4	0.000612	0.498416	0.877160
O21	0.876224	0.623677	-0.000252	FeA11	0.875081	0.751197	0.065089
O22	0.876782	0.123902	0.000027	FeA12	0.877826	0.251836	0.064791
O23	0.623668	0.623470	0.503060	FeA13	0.624775	0.752484	0.437839
O24	0.625675	0.124766	0.501602	FeA14	0.626440	0.253582	0.437797
O31	0.877520	0.870194	0.252412	FeA21	0.874646	0.504293	0.190011
O32	0.874280	0.375918	0.254608	FeA22	0.880150	0.000666	0.188405
O33	0.628978	0.876719	0.246166	FeA23	0.625237	0.501458	0.311231
O34	0.624928	0.370320	0.246103	FeA24	0.628806	0.004522	0.312748
O41	0.877088	0.636241	0.254284	FeB1A1	0.750513	-0.001908	0.002046
O42	0.877709	0.131021	0.251620	FeB1A2	0.751044	0.498785	0.001003
O43	0.628942	0.631444	0.247129	FeB1B1	0.001683	0.500450	0.501530
O44	0.626872	0.135620	0.249325	FeB1B2	-0.002313	0.000684	0.497238
O5A1	0.744150	0.750450	0.129770	FeB2A1	0.747822	0.755752	0.252342
O5A2	0.748686	0.255796	0.129815	FeB2A2	0.758361	0.251977	0.253306
O5A3	0.752439	0.754662	0.372516	FeB2B1	0.002295	0.744348	0.751689
O5A4	0.755274	0.256633	0.374280	FeB2B2	0.001926	0.246292	0.751719
O5B1	0.009054	0.748137	0.628681	FeB31	0.876746	0.879005	0.379325
O5B2	0.004653	0.245410	0.630220	FeB32	0.876296	0.386226	0.380174
O5B3	-0.004635	0.746769	0.872453	FeB33	0.626467	0.885462	0.122098
O5B4	-0.002466	0.244951	0.871616	FeB34	0.628402	0.374659	0.123301
O6A1	0.743835	0.502475	0.125729	FeB41	0.875891	0.624838	0.376535
O6A2	0.750927	-0.000360	0.124784	FeB42	0.875387	0.130283	0.374428
O6A3	0.752151	0.502943	0.376368	FeB43	0.625594	0.627484	0.125756
O6A4	0.758658	0.004293	0.376530	FeB44	0.627592	0.125909	0.126365

Fe_3O_4 d=100%

Lattice constants:

8.4066581710000	8.4066581710000	0.0000000000000
-8.3787910930000	8.3787910930000	0.0000000000000
-0.0489246839200	-0.0489246839200	16.7750073100000

Fractional coordinates:

site	*x*	*y*	*z*	site	*x*	*y*	*z*
O1	0.875810	0.880430	0.000140	O6B1	0.010990	-0.002290	0.623720
O12	0.876070	0.380720	-0.001640	O6B2	0.002780	0.498700	0.626080
O13	0.626910	0.881860	0.505000	O6B3	-0.002840	-0.002230	0.876290
O14	0.625560	0.382800	0.505790	O6B4	0.000680	0.498240	0.877400
O21	0.876360	0.623530	-0.000280	FeA11	0.875090	0.751330	0.065377
O22	0.876980	0.123780	0.000030	FeA12	0.878140	0.252040	0.065046
O23	0.623520	0.623300	0.503400	FeA13	0.624750	0.752760	0.437877
O24	0.625750	0.124740	0.501780	FeA14	0.626600	0.253980	0.437830
O31	0.877800	0.869660	0.252680	FeA21	0.874607	0.504770	0.190290
O32	0.874200	0.376020	0.255120	FeA22	0.880722	0.000740	0.188506
O33	0.629420	0.876910	0.245740	FeA23	0.625263	0.501620	0.311090
O34	0.624920	0.369800	0.245670	FeA24	0.629229	0.005024	0.312775
O41	0.877320	0.637490	0.254760	FeB1A1	0.750570	-0.002120	0.002273
O42	0.878010	0.131690	0.251800	FeB1A2	0.751160	0.498650	0.001114
O43	0.629380	0.632160	0.246810	FeB1B1	0.001870	0.500500	0.501700
O44	0.627080	0.136800	0.249250	FeB1B2	-0.002570	0.000760	0.496931
O5A1	0.743500	0.750500	0.130300	FeB2A1	0.747580	0.756391	0.252602
O5A2	0.748540	0.256440	0.130350	FeB2A2	0.759290	0.252197	0.253673
O5A3	0.752710	0.755180	0.372240	FeB2B1	0.002550	0.743720	0.751877
O5A4	0.755860	0.257370	0.374200	FeB2B2	0.002140	0.245880	0.751910
O5B1	0.010060	0.747930	0.629090	FeB31	0.876940	0.879450	0.379805
O5B2	0.005170	0.244900	0.630800	FeB32	0.876440	0.387473	0.380749
O5B3	-0.005150	0.746410	0.872170	FeB33	0.626630	0.886624	0.121776
O5B4	-0.002740	0.244390	0.871240	FeB34	0.628780	0.374621	0.123112
O6A1	0.743150	0.502750	0.125810	FeB41	0.875990	0.624820	0.376706
O6A2	0.751030	-0.000400	0.124760	FeB42	0.875430	0.130870	0.374365
O6A3	0.752390	0.503270	0.376520	FeB43	0.625660	0.627760	0.125840
O6A4	0.759620	0.004770	0.376700	FeB44	0.627880	0.126010	0.126517

<u>Section IV.</u> Lattice structure and crystallographic sites of low-temperature phase Fe_3O_4

Figure S5 shows the distribution of different Fe_B sites in monoclinic unit cell. The equivalent Fe_B ions are mark with same color. It should be noted that the charge ordering occurs at Fe_B sites. So, only the Fe_B sites are colored for easy viewing.

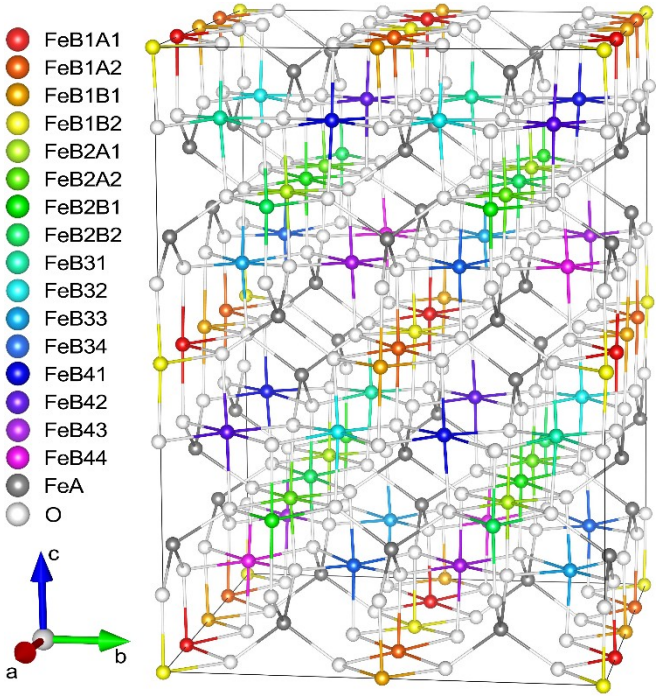

Fig. S5 Sketch map of monoclinic Fe_3O_4. The white and grey spheres represent O and Fe_A ions, respectively. Fe_B ions at different sites are marked with different colors.

References

1 H. T. Jeng, G. Y. Guo, and D. J. Huang, Charge-orbital ordering in low-temperature structures of magnetite: GGA+*U* investigations, *Phys. Rev. B*, 2006, **74**, 195115.

2 M. S. Senn, J. P. Wright, and J. P. Attfield, Charge order and three-site distortions in the Verwey structure of magnetite, *Nature*, 2012, **481**, 173-176.