Supplementary Material for

A metastable Fo-III wedge in cold slabs subducted to the lower part of the mantle transition zone: A hypothesis based on first-principles simulations

Yining Zhang[1,2,3], Yanyao Zhang[1,2], Yun Liu[3], Xi Liu[1,2,*]

[1]The Key Laboratory of Orogenic Belts and Crustal Evolution, Ministry of Education of China, Beijing 100871, China

[2]School of Earth and Space Sciences, Peking University, Beijing 100871, China

[3]State Key Laboratory of Ore Deposit Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550002, China

[*]Corresponding author. *E-mail address*: xi.liu@pku.edu.cn

List of Supplementary Tables

Fo, 0 GPa			
a (Å)	4.7866		
b (Å)	10.2732		
c (Å)	6.0188		
α (°)	90		
β (°)	90		
γ (°)	90		
V (Å^3)	295.96		
atom	x	y	z
Mg1	0.0000	0.0000	0.0000
Mg2	0.5000	0.5000	0.0000
Mg3	0.0000	0.0000	0.5000
Mg4	0.5000	0.5000	0.5000
Mg5	0.9917	0.2772	0.2500
Mg6	0.0083	0.7228	0.7500
Mg7	0.4917	0.2228	0.7500
Mg8	0.5083	0.7772	0.2500
Si1	0.4266	0.0937	0.2500
Si2	0.5735	0.9063	0.7500
Si3	0.9266	0.4063	0.7500
Si4	0.0735	0.5937	0.2500
O1	0.2768	0.1630	0.0324
O2	0.7232	0.8370	0.9677
O3	0.7768	0.3370	0.9677
O4	0.2232	0.6630	0.0324
O5	0.7232	0.8370	0.5324
O6	0.2768	0.1630	0.4677
O7	0.2232	0.6630	0.4677
O8	0.7768	0.3370	0.5324
O9	0.7672	0.0915	0.2500
O10	0.2328	0.9085	0.7500
O11	0.2672	0.4085	0.7500
O12	0.7328	0.5915	0.2500
O13	0.2225	0.4464	0.2500
O14	0.7775	0.5536	0.7500
O15	0.7225	0.0536	0.7500
O16	0.2775	0.9464	0.2500

Supplementary Table S1. Fo at 0 GPa (0K; GGA). Mg(I): Mg1-Mg4; Mg(II): Mg5-Mg8.

Fo-II, 0 GPa			
a (Å)	5.0838		
b (Å)	10.0037		
c (Å)	5.7633		
α (°)	92.063		
β (°)	107.649		
γ (°)	99.216		
V (Å^3)	274.58		
atom	x	y	z
Mg1	0.9871	0.1108	0.6835
Mg2	0.0260	0.9213	0.0143
Mg3	0.0079	0.6591	0.7331
Mg4	0.5066	0.5160	0.8489
Mg5	0.5532	0.7945	0.1504
Mg6	0.0052	0.3729	0.9647
Mg7	0.4599	0.2375	0.5474
Mg8	0.5066	0.5160	0.3489
Si1	0.9978	0.3869	0.4535
Si2	0.0153	0.6451	0.2443
Si3	0.6249	0.1214	0.0964
Si4	0.3882	0.9107	0.6014
O1	0.2758	0.8309	0.8109
O2	0.8014	0.6951	0.9716
O3	0.7586	0.2242	0.3732
O4	0.2634	0.0492	0.5362
O5	0.7373	0.2012	0.8869
O6	0.2117	0.3370	0.7262
O7	0.2545	0.8078	0.3246
O8	0.7934	0.6884	0.3980
O9	0.7960	0.4660	0.1774
O10	0.7497	0.9829	0.1616
O11	0.2171	0.5660	0.5204
O12	0.7725	0.4460	0.6362
O13	0.2844	0.0956	0.0214
O14	0.2406	0.5860	0.0616
O15	0.2197	0.3437	0.2998
O16	0.7287	0.9364	0.6764

Supplementary Table S2. Fo-II at 0 GPa (0K; GGA). Si(I): Si3-Si4; Si(II): Si1-Si2; Mg(I): Mg1-Mg2; Mg(II): Mg3, Mg6; Mg(III): Mg4; Mg(IV): Mg5, Mg7; Mg(V): Mg8.

Fo-II, 60 GPa			
a (Å)	4.6785		
b (Å)	9.1887		
c (Å)	5.2943		
α (°)	93.247		
β (°)	106.994		
γ (°)	97.782		
V (Å^3)	214.54		
atom	x	y	z
Mg1	0.9716	0.0965	0.6402
Mg2	0.0415	0.9355	0.0576
Mg3	0.0012	0.6657	0.7355
Mg4	0.5066	0.5160	0.8489
Mg5	0.5350	0.7885	0.1357
Mg6	0.0119	0.3664	0.9623
Mg7	0.4781	0.2435	0.5621
Mg8	0.5066	0.5160	0.3489
Si1	0.0065	0.3874	0.4588
Si2	0.0066	0.6446	0.2390
Si3	0.6118	0.1219	0.0943
Si4	0.4013	0.9101	0.6034
O1	0.2669	0.8422	0.8232
O2	0.7788	0.6995	0.9616
O3	0.7652	0.2267	0.3772
O4	0.2748	0.0520	0.4862
O5	0.7462	0.1898	0.8746
O6	0.2343	0.3325	0.7361
O7	0.2479	0.8053	0.3206
O8	0.7754	0.6952	0.4051
O9	0.7886	0.4603	0.1706
O10	0.7383	0.9800	0.2116
O11	0.2245	0.5718	0.5272
O12	0.7748	0.4488	0.6486
O13	0.2598	0.1101	0.9975
O14	0.2383	0.5832	0.0492
O15	0.2377	0.3368	0.2927
O16	0.7533	0.9219	0.7003

Supplementary Table S3. Fo-II at 60 GPa (0K; GGA). Si(I): Si3-Si4; Si(II): Si1-Si2; Mg(I): Mg1-Mg2; Mg(II): Mg3, Mg6; Mg(III): Mg4; Mg(IV): Mg5, Mg7; Mg(V): Mg8.

Fo-III, 0 GPa			
a (Å)	2.7923		
b (Å)	9.4664		
c (Å)	9.4266		
α (°)	90		
β (°)	90		
γ (°)	90		
V (Å^3)	249.17		
atom	x	y	z
Mg1	0.5000	0.3608	0.3547
Mg2	0.5000	0.6392	0.8547
Mg3	0.0000	0.8608	0.3547
Mg4	0.0000	0.1392	0.8547
Mg5	0.5000	0.8923	0.6876
Mg6	0.5000	0.1078	0.1876
Mg7	0.0000	0.3923	0.6876
Mg8	0.0000	0.6078	0.1876
Si1	0.0000	0.8731	0.0000
Si2	0.0000	0.1269	0.5000
Si3	0.5000	0.3731	0.0000
Si4	0.5000	0.6269	0.5000
O1	0.5000	0.0056	0.4377
O2	0.5000	0.9944	0.9377
O3	0.0000	0.5056	0.4377
O4	0.0000	0.4944	0.9377
O5	0.5000	0.2473	0.5463
O6	0.5000	0.7527	0.0463
O7	0.0000	0.7473	0.5463
O8	0.0000	0.2527	0.0463
O9	0.5000	0.7054	0.3270
O10	0.5000	0.2946	0.8270
O11	0.0000	0.2054	0.3270
O12	0.0000	0.7946	0.8270
O13	0.5000	0.4553	0.1634
O14	0.5000	0.5447	0.6634
O15	0.0000	0.9553	0.1634
O16	0.0000	0.0447	0.6634

Supplementary Table S4. Fo-III at 0 GPa (0K; GGA). Mg(I): Mg1-Mg4; Mg(II): Mg5-Mg8.

Fo-III, 60 GPa			
a (Å)	2.6305		
b (Å)	8.8223		
c (Å)	8.9048		
α (°)	90		
β (°)	90		
γ (°)	90		
V (Å^3)	206.65		
atom	x	y	z
Mg1	0.5000	0.3636	0.3548
Mg2	0.5000	0.6364	0.8548
Mg3	0.0000	0.8636	0.3548
Mg4	0.0000	0.1364	0.8548
Mg5	0.5000	0.8861	0.6799
Mg6	0.5000	0.1139	0.1799
Mg7	0.0000	0.3861	0.6799
Mg8	0.0000	0.6139	0.1799
Si1	0.0000	0.8719	0.0000
Si2	0.0000	0.1281	0.5000
Si3	0.5000	0.3719	0.0000
Si4	0.5000	0.6281	0.5000
O1	0.5000	0.0034	0.4402
O2	0.5000	0.9966	0.9402
O3	0.0000	0.5034	0.4402
O4	0.0000	0.4966	0.9402
O5	0.5000	0.2559	0.5497
O6	0.5000	0.7441	0.0497
O7	0.0000	0.7559	0.5497
O8	0.0000	0.2441	0.0497
O9	0.5000	0.7068	0.3237
O10	0.5000	0.2932	0.8237
O11	0.0000	0.2068	0.3237
O12	0.0000	0.7932	0.8237
O13	0.5000	0.4544	0.1672
O14	0.5000	0.5456	0.6672
O15	0.0000	0.9544	0.1672
O16	0.0000	0.0456	0.6672

Supplementary Table S5. Fo-III at 60 GPa (0K; GGA). Mg(I): Mg1-Mg4; Mg(II): Mg5-Mg8.

Fo-IV, 0 GPa			
a (Å)	10.0545		
b (Å)	5.1286		
c (Å)	5.0421		
α (°)	90		
β (°)	90		
γ (°)	90		
V (Å^3)	260.00		
atom	x	y	z
Mg1	0.0790	0.2935	0.7498
Mg2	0.9210	0.7065	0.7498
Mg3	0.4210	0.7935	0.2502
Mg4	0.5790	0.2065	0.2502
Mg5	0.7473	0.1600	0.7413
Mg6	0.2527	0.8400	0.7413
Mg7	0.7527	0.6600	0.2587
Mg8	0.2473	0.3400	0.2587
Si1	0.9300	0.2090	0.2331
Si2	0.0700	0.7910	0.2331
Si3	0.5700	0.7090	0.7669
Si4	0.4300	0.2910	0.7669
O1	0.7276	0.7723	0.6354
O2	0.2724	0.2277	0.6354
O3	0.7724	0.2723	0.3646
O4	0.2276	0.7277	0.3646
O5	0.6087	0.8514	0.0708
O6	0.3913	0.1486	0.0708
O7	0.8913	0.3514	0.9292
O8	0.1087	0.6486	0.9292
O9	0.1015	0.1201	0.1109
O10	0.8985	0.8799	0.1109
O11	0.3985	0.6201	0.8891
O12	0.6015	0.3799	0.8891
O13	0.5000	0.0000	0.6012
O14	0.0000	0.5000	0.3988
O15	0.5000	0.5000	0.4822
O16	0.0000	0.0000	0.5178

Supplementary Table S6. Fo-IV at 0 GPa (0K; GGA). Mg(I): Mg1-Mg4; Mg(II): Mg5-Mg8.

Fo-IV, 20 GPa			
a (Å)	9.6786		
b (Å)	5.0276		
c (Å)	4.8181		
α (°)	90		
β (°)	90		
γ (°)	90		
V (Å^3)	234.45		
atom	x	y	z
Mg1	0.0791	0.2994	0.7433
Mg2	0.9209	0.7006	0.7433
Mg3	0.4209	0.7994	0.2568
Mg4	0.5791	0.2006	0.2568
Mg5	0.7469	0.1365	0.7614
Mg6	0.2531	0.8635	0.7614
Mg7	0.7531	0.6365	0.2386
Mg8	0.2469	0.3635	0.2386
Si1	0.9287	0.2059	0.2390
Si2	0.0713	0.7941	0.2390
Si3	0.5713	0.7059	0.7611
Si4	0.4287	0.2941	0.7611
O1	0.7301	0.7632	0.6208
O2	0.2699	0.2368	0.6208
O3	0.7699	0.2632	0.3792
O4	0.2301	0.7368	0.3792
O5	0.6129	0.8602	0.0654
O6	0.3871	0.1398	0.0654
O7	0.8871	0.3602	0.9346
O8	0.1129	0.6398	0.9346
O9	0.1043	0.1184	0.1035
O10	0.8957	0.8816	0.1035
O11	0.3957	0.6184	0.8965
O12	0.6043	0.3816	0.8965
O13	0.5000	0.0000	0.5958
O14	0.0000	0.5000	0.4042
O15	0.5000	0.5000	0.4752
O16	0.0000	0.0000	0.5248

Supplementary Table S7. Fo-IV at 20 GPa (0K; GGA). Mg(I): Mg1-Mg4; Mg(II): Mg5-Mg8..

Fo-IV, 40 GPa			
a (Å)	9.4041		
b (Å)	4.9571		
c (Å)	4.6718		
α (°)	90		
β (°)	90		
γ (°)	90		
V (Å^3)	217.79		
atom	x	y	z
Mg1	0.0787	0.3023	0.7409
Mg2	0.9213	0.6978	0.7409
Mg3	0.4213	0.8023	0.2591
Mg4	0.5787	0.1978	0.2591
Mg5	0.7476	0.1229	0.7729
Mg6	0.2525	0.8771	0.7729
Mg7	0.7525	0.6229	0.2271
Mg8	0.2476	0.3771	0.2271
Si1	0.9284	0.2045	0.2426
Si2	0.0716	0.7955	0.2426
Si3	0.5716	0.7045	0.7574
Si4	0.4284	0.2955	0.7574
O1	0.7316	0.7589	0.6113
O2	0.2684	0.2411	0.6113
O3	0.7684	0.2589	0.3887
O4	0.2316	0.7411	0.3887
O5	0.6149	0.8639	0.0638
O6	0.3851	0.1361	0.0638
O7	0.8851	0.3639	0.9362
O8	0.1149	0.6361	0.9362
O9	0.1066	0.1172	0.1002
O10	0.8934	0.8828	0.1002
O11	0.3934	0.6172	0.8998
O12	0.6066	0.3828	0.8998
O13	0.5000	0.0000	0.5950
O14	0.0000	0.5000	0.4050
O15	0.5000	0.5000	0.4690
O16	0.0000	0.0000	0.5310

Supplementary Table S8. Fo-IV at 40 GPa (0K; GGA). Mg(I): Mg1-Mg4; Mg(II): Mg5-Mg8.

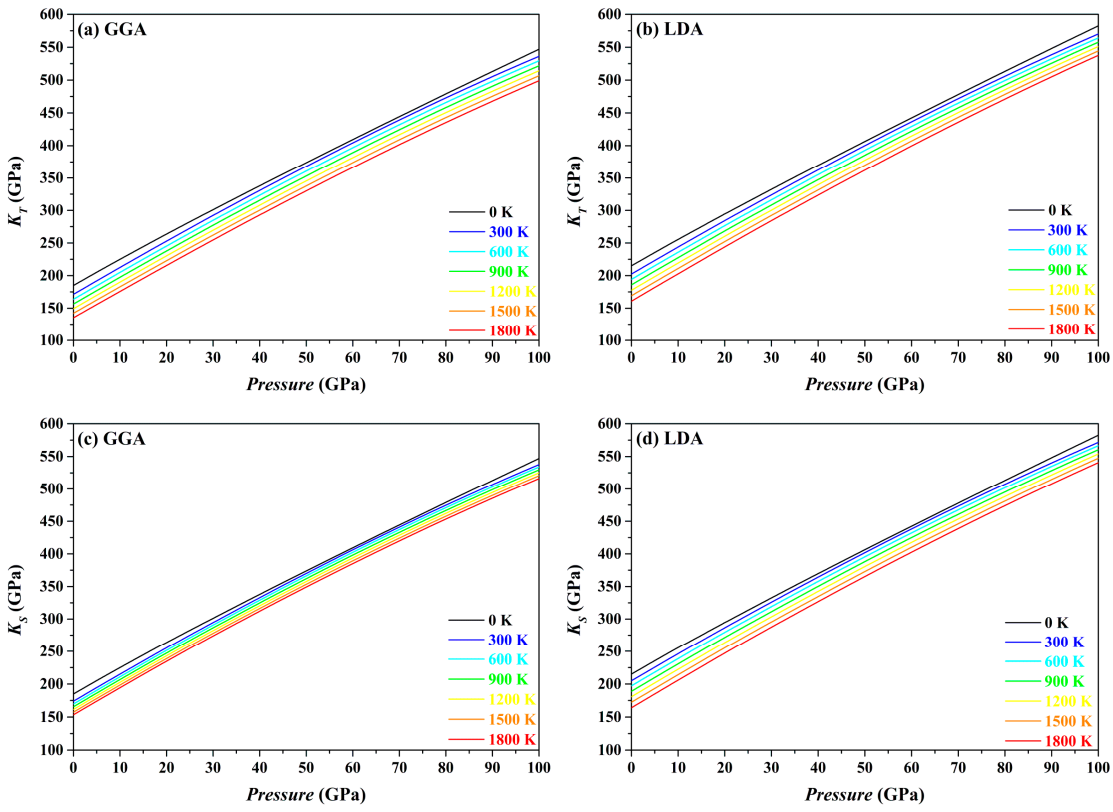
List of Supplementary Figures

Supplementary Figure S1. Calculated K_T and K_S of Fo-III at 0, 300, 600, 900, 1200, 1500 and 1800 K from 0 to 100 GPa using both GGA and LDA methods.

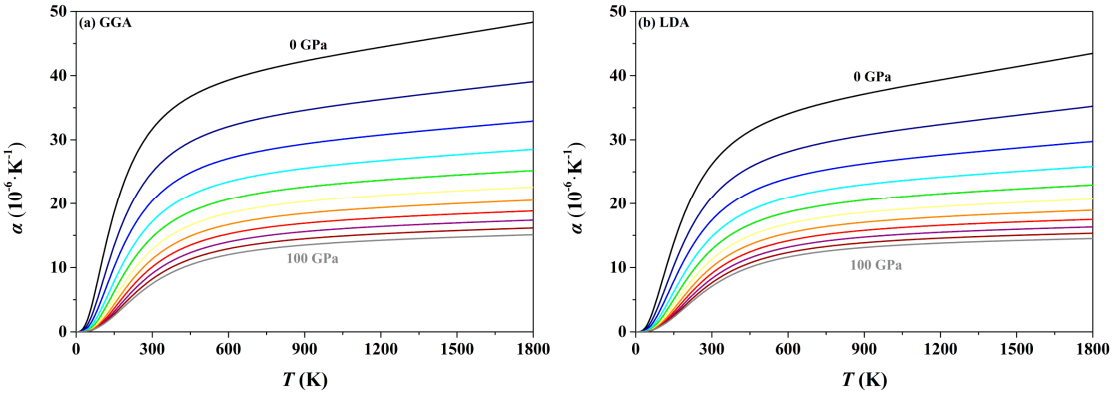
Supplementary Figure S2. Calculated α of Fo-III from 0 to 1800 K at 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GPa using both GGA and LDA methods.

Supplementary Figure S3. Calculated γ_{th} of Fo-III from 0 to 1800 K at 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GPa using both GGA and LDA methods.

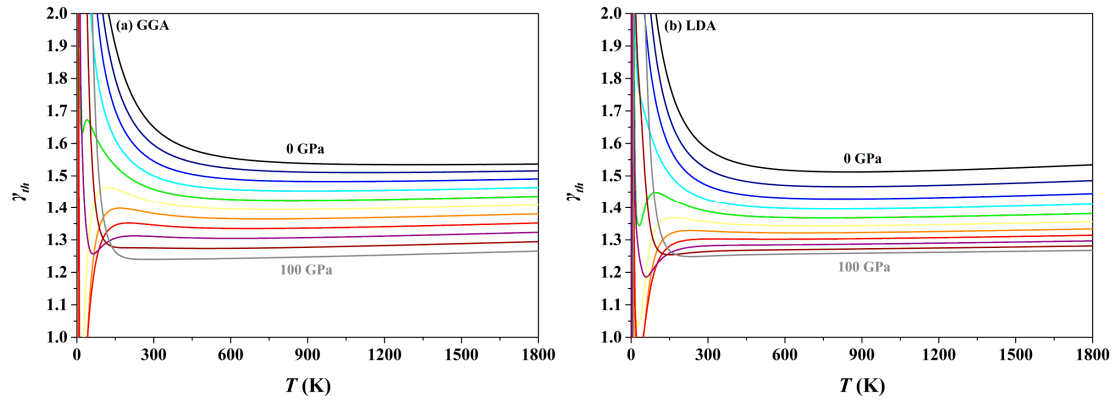
Supplementary Figure S4. Calculated C_V and C_P of Fo-III from 0 to 1800 K at 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GPa using both GGA and LDA methods



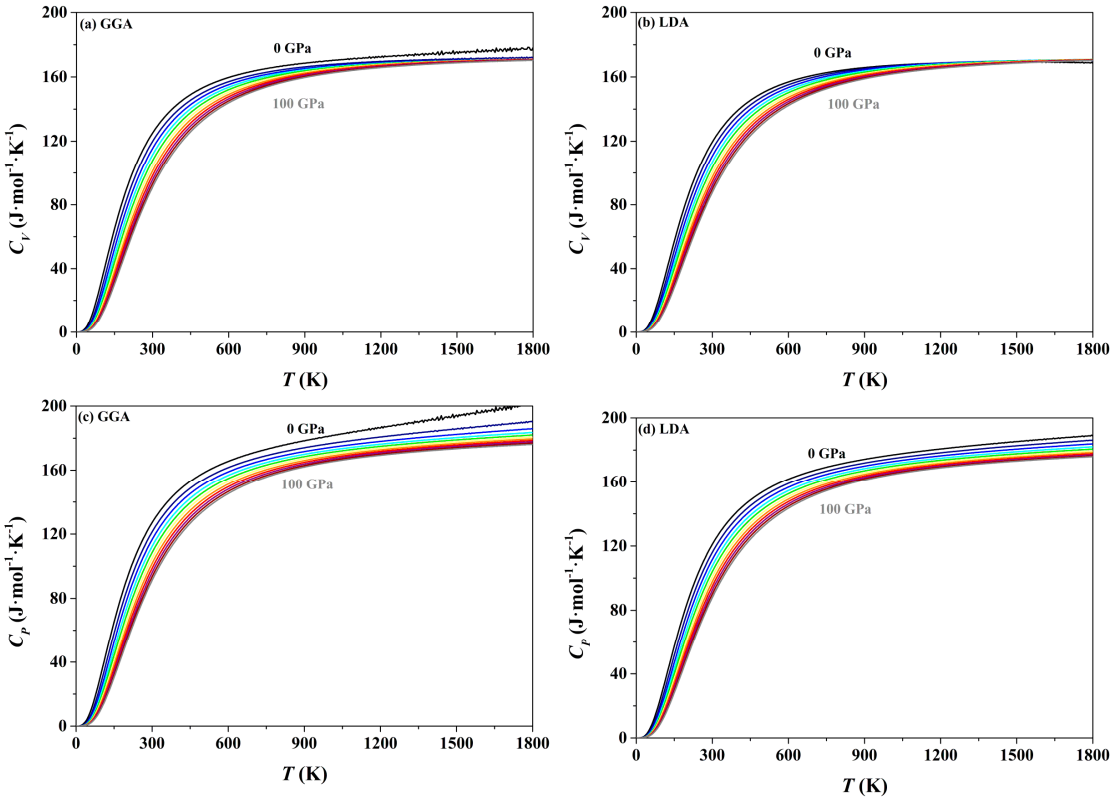
Supplementary Figure S1. Calculated K_T and K_S of Fo-III at 0, 300, 600, 900, 1200, 1500 and 1800 K from 0 to 100 GPa using both GGA and LDA methods.



Supplementary Figure S2. Calculated α of Fo-III from 0 to 1800 K at 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GPa using both GGA and LDA methods.



Supplementary Figure S3. Calculated γ_{th} of Fo-III from 0 to 1800 K at 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GPa using both GGA and LDA methods.



Supplementary Figure S4. Calculated C_V and C_P of Fo-III from 0 to 1800 K at 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 GPa using both GGA and LDA methods