Supplementary Information for X-raying $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$: disentangling elemental contributions in a prototypical high-entropy oxide

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I. NUMERICAL RESULTS OF THE EXAFS FITS

Tables I–XI report the complete set of EXAFS fitting parameters obtained for the 5HEO, noMg, and noCu samples at the Cu, Ni, and Co K edges. Among these, Tables VII and VIII are also presented in the main text for clarity.

shell	atom	(Å)	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O		6	2.03(1)	0.012(2)	-0.12(6)	0.0016(2)
2	M		12	3.000(9)	0.012(1)		
3	O		8	3.25(1)	0.002(2)		
4	M		6	3.82(1)	0.027(7)		
5	O		24	4.27(1)	0.003(1)		
6	M		24	4.71(2)	0.014(2)		
7	M		12	5.57(4)	0.014(6)		

TABLE I. EXAFS fitted parameters for the data at the Co K edge for the noCu sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

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shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	1.95(2)	0.025(2)	-0.04(4)	0.0039(2)
2	M	12	2.987(9)	0.016(2)		
3	O	8	3.25(2)	0.006(2)		
4	M	6	3.70(3)	0.029(7)		
5	O	24	4.1(1)	0.04(6)		
6	M	24	4.69(4)	0.025(4)		
7	M	12	5.54(3)	0.015(3)		

TABLE II. EXAFS fitted parameters for the data at the Cu K edge for the noMg sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.02(1)	0.011(2)	-0.16(6)	0.0014(3)
2	M	12	3.01(1)	0.012(1)		
3	O	8	3.26(1)	0.001(2)		
4	M	6	3.83(1)	0.026(7)		
5	O	24	4.27(1)	0.004(1)		
6	M	24	4.72(3)	0.015(3)		
7	M	12	5.52(2)	0.008(2)		

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TABLE III. EXAFS fitted parameters for the data at the Ni K edge for the noCu sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.08(1)	0.010(2)		
2	M	12	3.013(6)	0.011(1)		
3	O	8	3.27(1)	0.006(2)		
4	M	6	4.09(3)	0.08(10)		
5	O	24	4.71(3)	0.008(4)		
6	M	24	5.17(2)	0.014(2)		
7	M	12	6.11(2)	0.007(2)		

TABLE IV. EXAFS fitted parameters for the data at the Co K edge for the HEO sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.08(1)	0.011(2)		
2	M	12	3.012(6)	0.011(1)		
3	O	8	3.25(1)	0.003(2)		
4	M	6	4.23(1)	0.012(1)		
5	O	24	4.64(3)	0.008(3)		
6	M	24	5.17(1)	0.011(2)		
7	M	12	6.11(2)	0.065(2)		

TABLE V. EXAFS fitted parameters for the data at the Co K edge for the noCu sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.09(1)	0.013(2)		
2	M	12	3.005(5)	0.010(1)		
3	O	8	3.30(1)	0.006(2)		
4	M	6	4.20(2)	0.020(5)		
5	O	24	4.71(4)	0.011(5)		
6	M	24	5.18(1)	0.013(2)		
7	M	12	6.14(2)	0.007(2)		

TABLE VI. EXAFS fitted parameters for the data at the Co K edge for the noMg sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.01(1)	0.013(2)		0.00300(9)
2	M	12	3.009(6)	0.011(1)		
3	O	8	3.26(1)	0.005(2)		
4	M	6	4.21(1)	0.016(2)		
5	O	24	3.97(4)	0.015(5)		
6	M	24	5.19(2)	0.015(2)		
7	M	12	5.5(2)	0.03(2)		

TABLE VII. EXAFS fitted parameters for the data at the Cu K edge for the HEO sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	1.987(6)	0.024(1)		0.003987(2)
2	M	12	3.001(6)	0.014(1)		
3	O	8	3.28(1)	0.008(3)		
4	M	6	4.17(5)	0.028(7)		
5	O	24	3.96(5)	0.020(8)		
6	M	24	5.19(3)	0.019(3)		
7	M	12	5.51(4)	0.017(6)		

TABLE VIII. EXAFS fitted parameters for the data at the Cu K edge for the noMg sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.074(8)	0.008(1)		
2	M	12	3.012(5)	0.010(2)		
3	O	8	3.27(1)	0.004(2)		
4	M	6	4.22(2)	0.016(3)		
5	O	24	4.812(3)	0.03(5)		
6	M	24	5.18(1)	0.012(2)		
7	M	12	5.74(4)	0.013(5)		

TABLE IX. EXAFS fitted parameters for the data at the Ni K edge for the HEO sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.11(1)	0.009(2)		
2	M	12	3.042(8)	0.009(1)		
3	O	8	3.26(2)	0.004(3)		
4	M	6	4.27(1)	0.011(2)		
5	O	24	4.82(5)	0.015(3)		
6	M	24	5.24(2)	0.012(2)		
7	M	12	5.82(4)	0.010(4)		

TABLE X. EXAFS fitted parameters for the data at the Ni K edge for the noCu sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

shell	atom	N	R (Å)	σ (Å^2)	b (Å^3)	c (Å^4)
1	O	6	2.14(1)	0.012(3)		
2	M	12	3.043(5)	0.009(1)		
3	O	8	4.0(2)	0.14(11)		
4	M	6	4.25(2)	0.016(3)		
5	O	24	4.79(4)	0.010(5)		
6	M	24	5.28(2)	0.014(3)		
7	M	12	5.86(2)	0.008(3)		

TABLE XI. EXAFS fitted parameters for the data at the Ni K edge for the noMg sample. N: coordination number; R: distance; σ^2: EXAFS Debye-Waller factors; b: skewness; c: kurtosis.

II. EXTENDED PDF DATA

Table XII reports the average interatomic distances derived from the lattice parameters for the 5HEO, noCu, and noMg samples. For comparison, it also shows the peak positions and widths obtained from single-peak fitting of the PDF data.

Atom pair	1st M–O	1st M–M	2nd M–O	2nd M–M	3rd M–O	3rd M–M
Length	$a/2$	$a\sqrt{2}/2$	$a\sqrt{3}/2$	a	$\sqrt{(a/2)^2+a^2}$	$\sqrt{(a\sqrt{2}/2)^2+a^2}$
Multiplicity	6	12	8	6	24	24
			5HEO			
Average distance (Å)	2.118	2.996	3.669	4.234	4.737	5.189
Local distance (Å)	2.090	2.974	3.664	4.190	4.687	5.146
FWHM (Å)	0.204	0.192	0.232	0.280	0.280	0.250
			noCu			
Average distance (Å)	2.115	2.991	3.663	4.230	4.729	5.181
Local distance (Å)	2.121	2.982	3.656	4.215	4.719	5.162
FWHM (Å)	0.172	0.194	0.176	0.242	0.228	0.225
			noMg			
Average distance (Å)	2.105 ×2	2.996 ×8	3.676 ×8	4.211 ×2	4.719 ×8	5.178 ×8
	2.131 ×4	3.0138 ×4		4.262 ×4	4.754 ×8	5.210 ×16
					4.765 ×8	
Local distance (Å)	2.120	2.990	3.675	4.216	4.721	5.173
FWHM (Å)	0.162	0.216	0.190	0.314	0.300	0.272

TABLE XII. Detailed information extracted from PDF data analyses.