Tracking of structural defects induced by Eu-doping in β-Ag_2MoO_4: their influences on electrical properties

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SUPPORTING INFORMATION

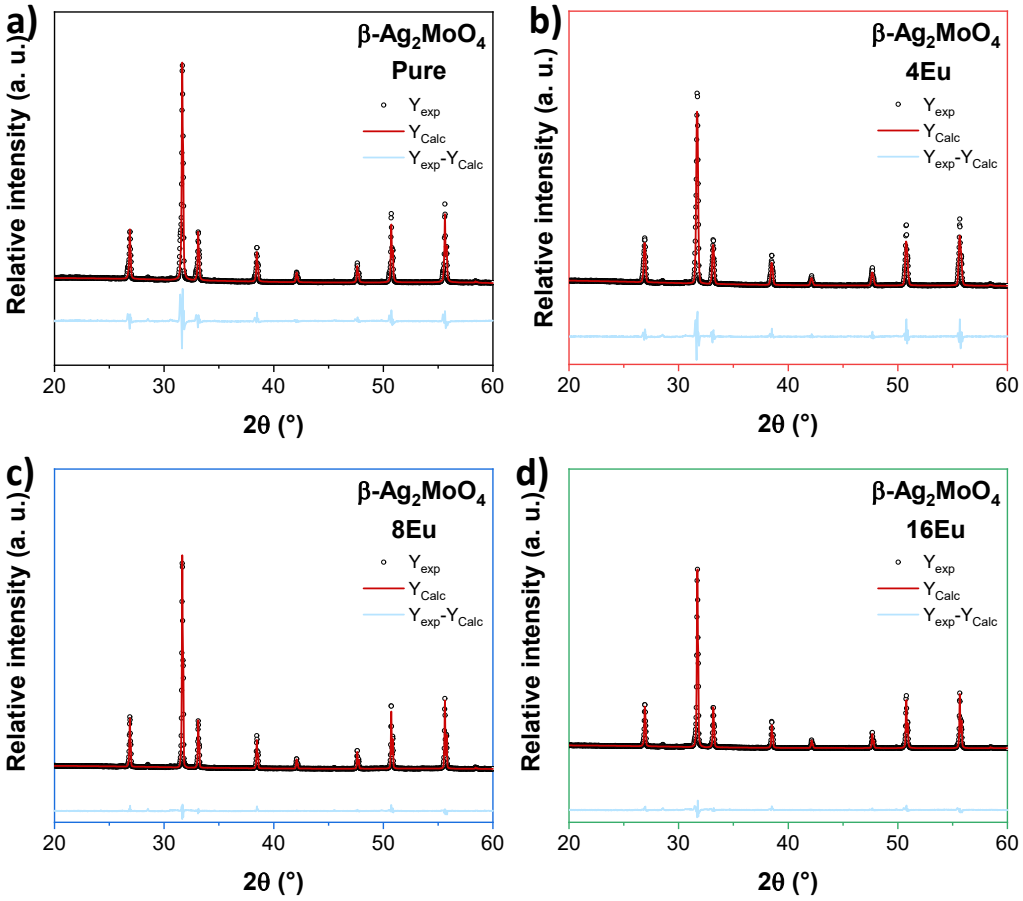

Figure S1 - Rietveld refinement fitting of the XRD for the samples a) Pure, b) 4Eu, c)8Eu, and d) 16Eu.

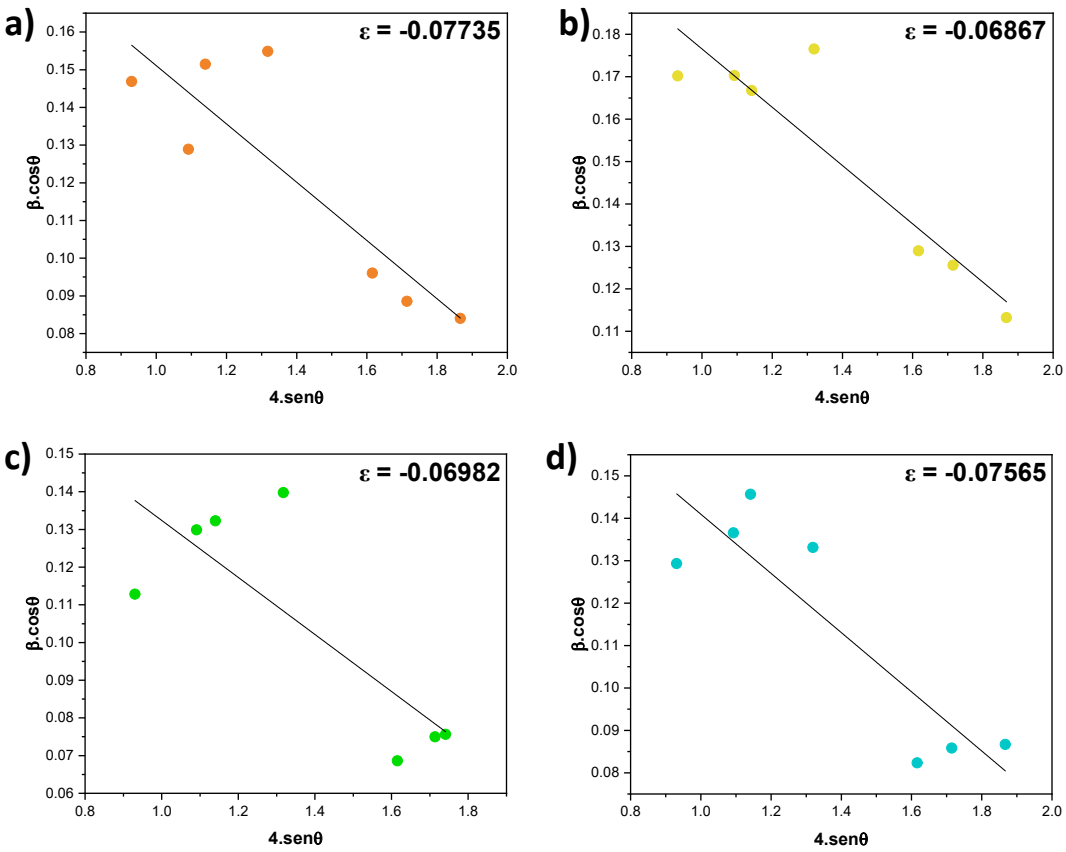

Figure S2 - Williamson-Hall plots for the samples a) Pure, b) 4Eu, c)8Eu, and d) 16Eu.

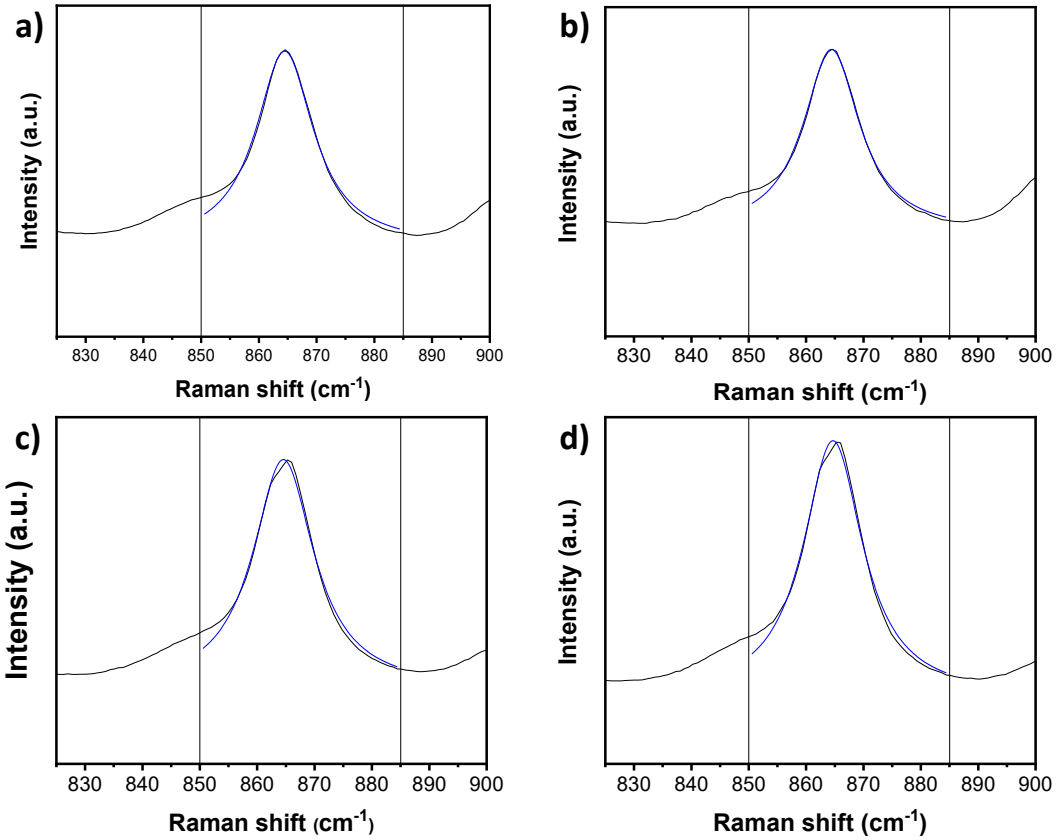

Figure S3 - Deconvolution of the A_{1g} Raman mode for the samples a) Pure, b) 4Eu, c)8Eu, and d) 16Eu.

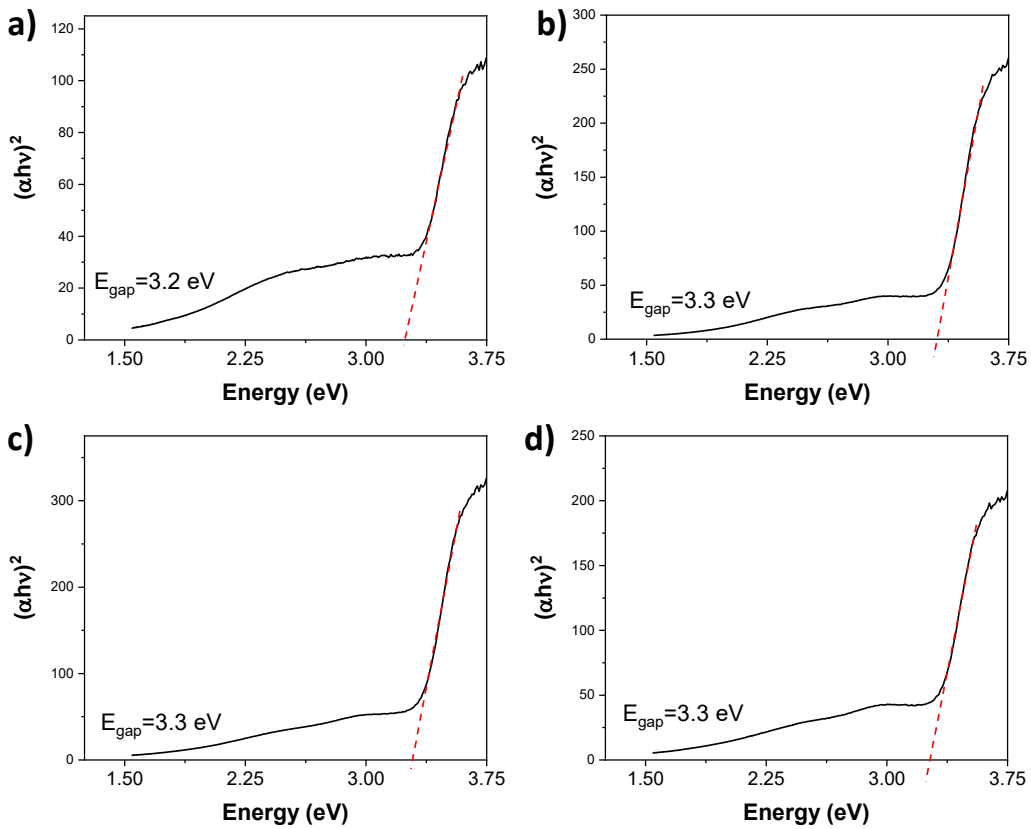

Figure S4 - E_{gap} determination for the samples a) Pure, b) 4Eu, c)8Eu, and d) 16Eu.

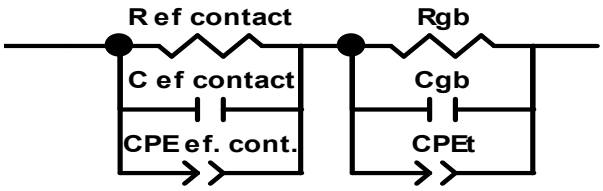

Figure S5 - Equivalent circuit model for theoretical adjustments of the data for the Nyquist plot combining ideal resistors, capacitors, and inductors. R_{ef} is the contact effective electrical resistance, C_{ef} is the contact effective electrical capacitance. R_{gb} is the grain boundary electrical resistance, C_{gb} is the is the grain boundary electrical capacitance. $CPE_{\text{ef contact}}$ is the Constant Phase Element (CPE) for the contact and CPE_t the Constant Phase Element (CPE) for the traps.

Table S1 - Rietveld refinement fitting and lattice parameters for all samples of the β-Ag_2MoO_4 system.

Sample	Lattice parameters		Rietveld parameters		
	V (Å^3)	phase (%)	R_{bragg}	R_{wp}	χ^2
Pure	806.73±10	100.0	3.63	12.14	3.55
4Eu	807.36±23	100.0	0.89	2.27	1.68
8Eu	807.54±80	100.0	1.16	0.86	0.77
16Eu	808.18±21	100.0	0.73	0.72	0.74

Table S2 - XRD and Raman FWHM for all samples of the β-Ag_2MoO_4 system.

Samples	XRD FWHM	Raman FWHM
Pure	0.14	9.8
4Eu	0.17	9.9
8Eu	0.12	10.8
16Eu	0.12	11.0

Table S3 – Atomic coordinates, occupancy factor and anisotropic thermal factor (B_{eq}).

	Site	Np	x	y	z	Atom	Occupancy	B_{eq}
Pure	Ag1	16	0.62500	0.62500	0.62500	Ag^{+}	0.99	3.91
	Eu1	16	0.62500	0.62500	0.62500	Eu^{3+}	0.01	0.01
	Mo1	8	0.00000	0.00000	0.00000	Mo^{6+}	1.00	1.99
	O1	32	0.36616	0.30897	0.36616	O^{2-}	1.00	20.0
	Site	Np	x	y	z	Atom	Occupancy	Beq
4Eu	Ag1	16	0.62500	0.62500	0.62500	Ag^{+}	0.99	2.75
	Eu1	16	0.62500	0.62500	0.62500	Eu^{3+}	0.01	0.03
	Mo1	8	0.00000	0.00000	0.00000	Mo^{6+}	1.00	1.13
	O1	32	0.32423	0.38366	0.32423	O^{2-}	1.00	19.9
	Site	Np	x	y	z	Atom	Occupancy	Beq
8Eu	Ag1	16	0.62500	0.62500	0.62500	Ag^{+}	0.99	3.37
	Eu1	16	0.62500	0.62500	0.62500	Eu^{3+}	0.01	0.01
	Mo1	8	0.00000	0.00000	0.00000	Mo^{6+}	1.00	1.59
	O1	32	0.32436	0.38437	0.32436	O^{2-}	1.00	19.9
	Site	Np	x	y	z	Atom	Occupancy	Beq
16Eu	Ag1	16	0.62500	0.62500	0.62500	Ag^{+}	0.99	3.39
	Eu1	16	0.62500	0.62500	0.62500	Eu^{3+}	0.01	0.12
	Mo1	8	0.00000	0.00000	0.00000	Mo^{6+}	1.00	1.72
	O1	32	0.32309	0.38490	0.32309	O^{2-}	1.00	19.9

Table S4 – CIE coordinates and CCT of the samples

Samples	x	y	CCT (K)	Color purity (%)
Pure	0.3832	0.3197	4800	-
4Eu	0.5042	0.3330	3964	30.73
8Eu	0.5213	0.3222	4886	36.46
16Eu	0.5501	0.3200	6130	43.98