Electronic Supplementary Material (ESI) for CrystEngComm.

Electrochemical performance and structure of $Al_2W_xMo_{3-x}O_{12}$

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Supporting Information

Structural Characterisation

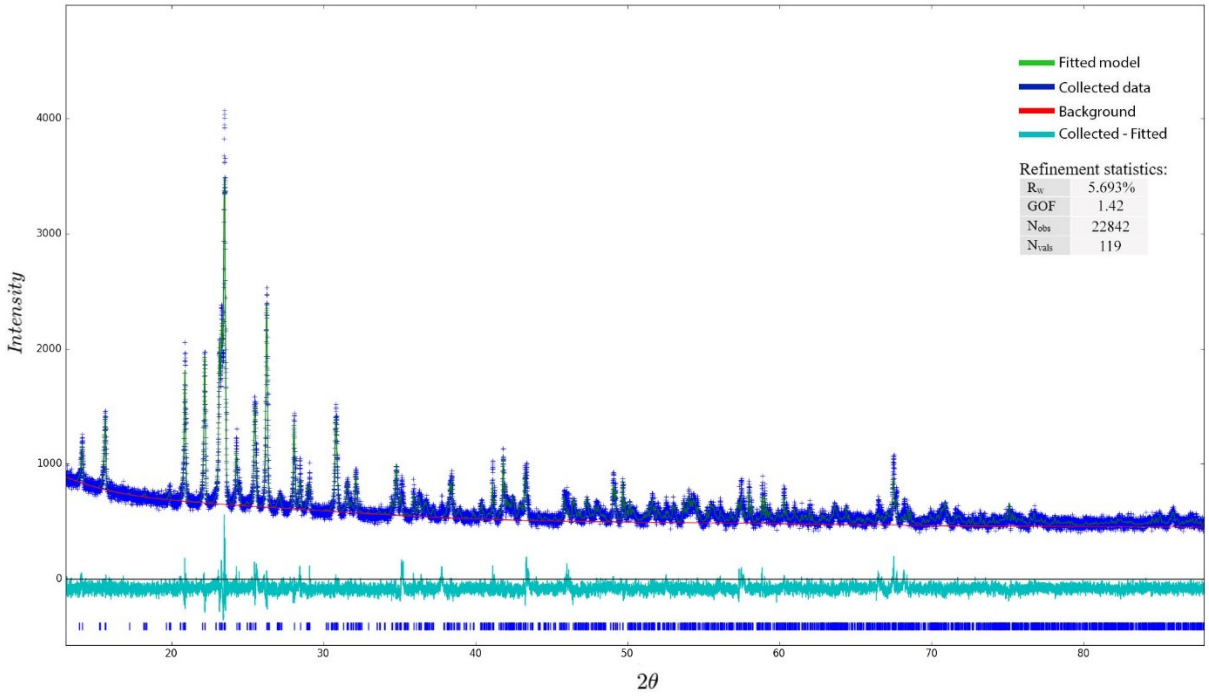

Figure S1 – Rietveld-refined fit of the $Al_2Mo_3O_{12}$ structural model to XRD data.

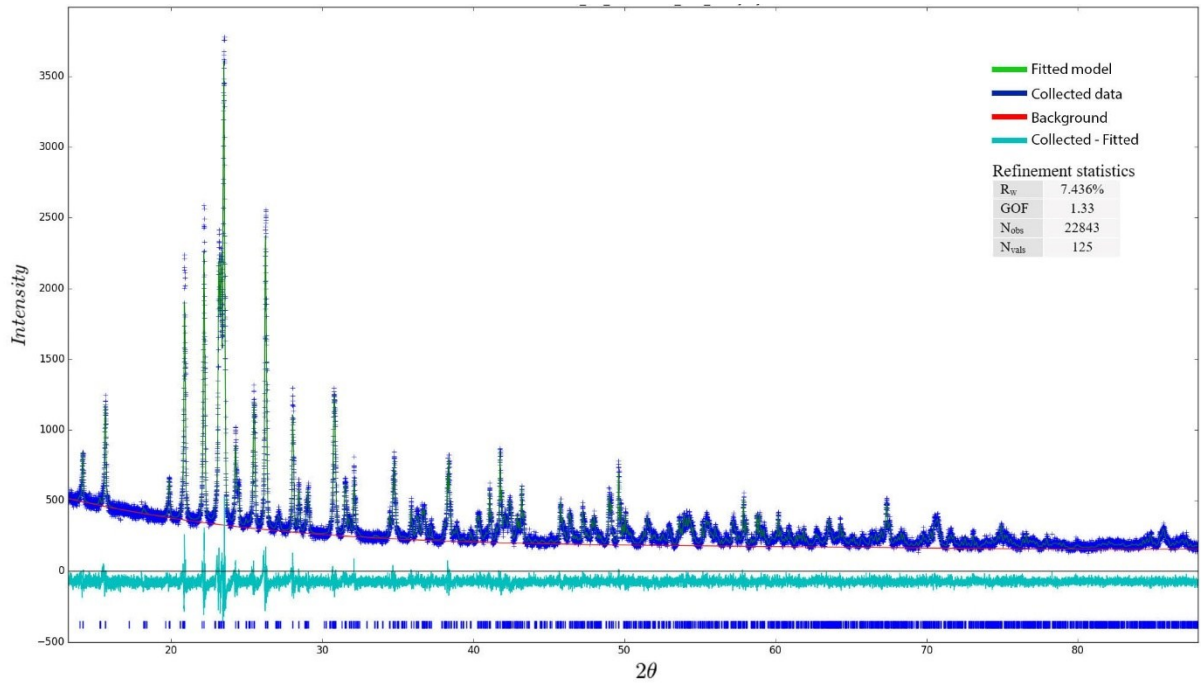

Figure S2 – Rietveld-refined fit of the $Al_2W_1Mo_2O_{12}$ ($Al_2W_{1.025}Mo_{1.975}O_{12}$) structural model to XRD data.

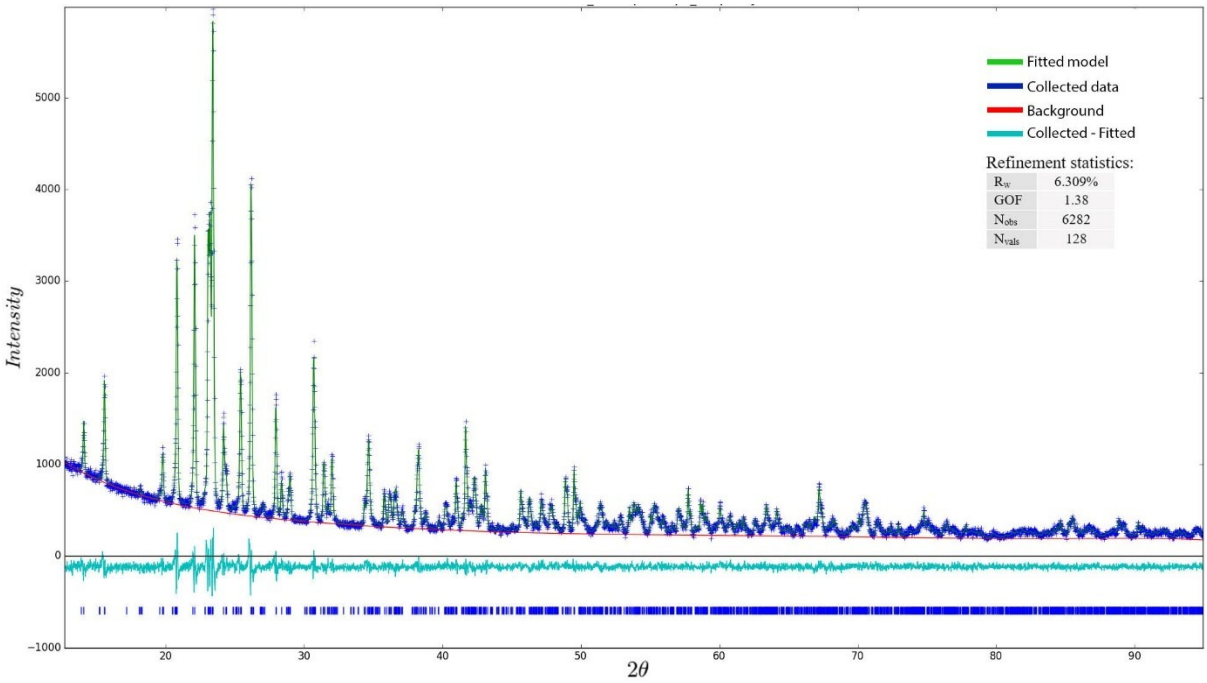

Figure S3 – Rietveld-refined fit of the $Al_2W_{1.5}Mo_{1.5}O_{12}$ ($Al_2W_{1.512}Mo_{1.488}O_{12}$) structural model to XRD data.

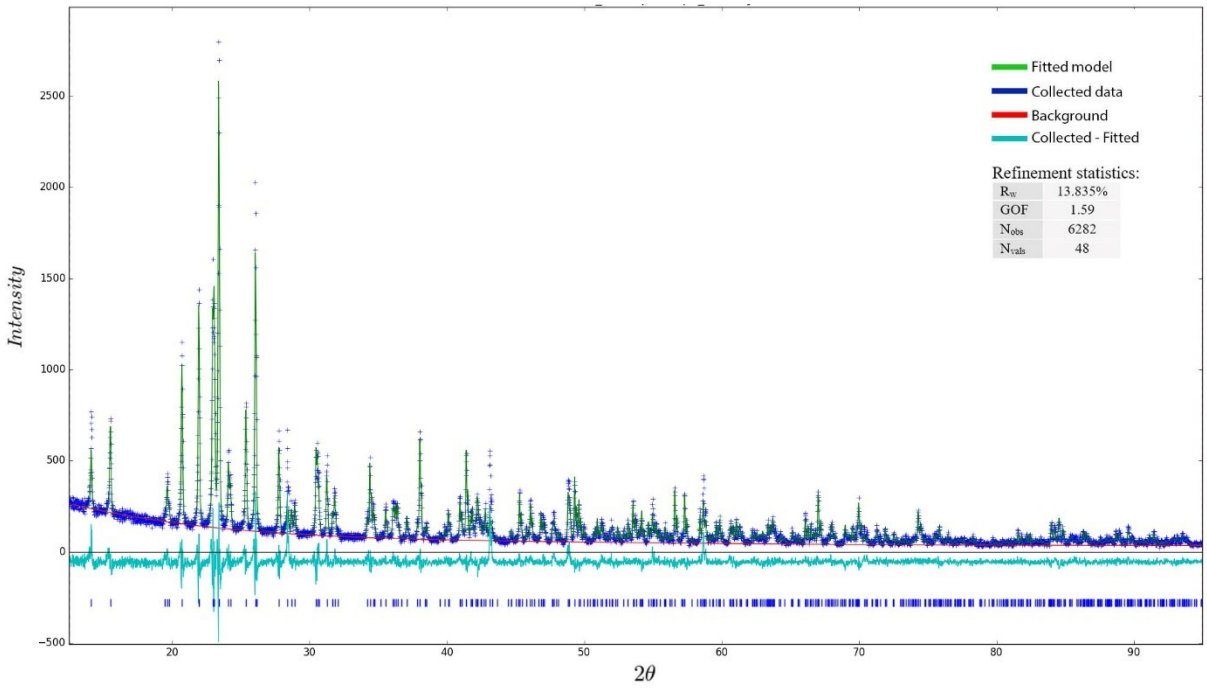

Figure S4 – Rietveld-refined fit of the $Al_2W_{2.5}Mo_{0.5}O_{12}$ ($Al_2W_{2.375}Mo_{0.625}O_{12}$) structural model to XRD data.

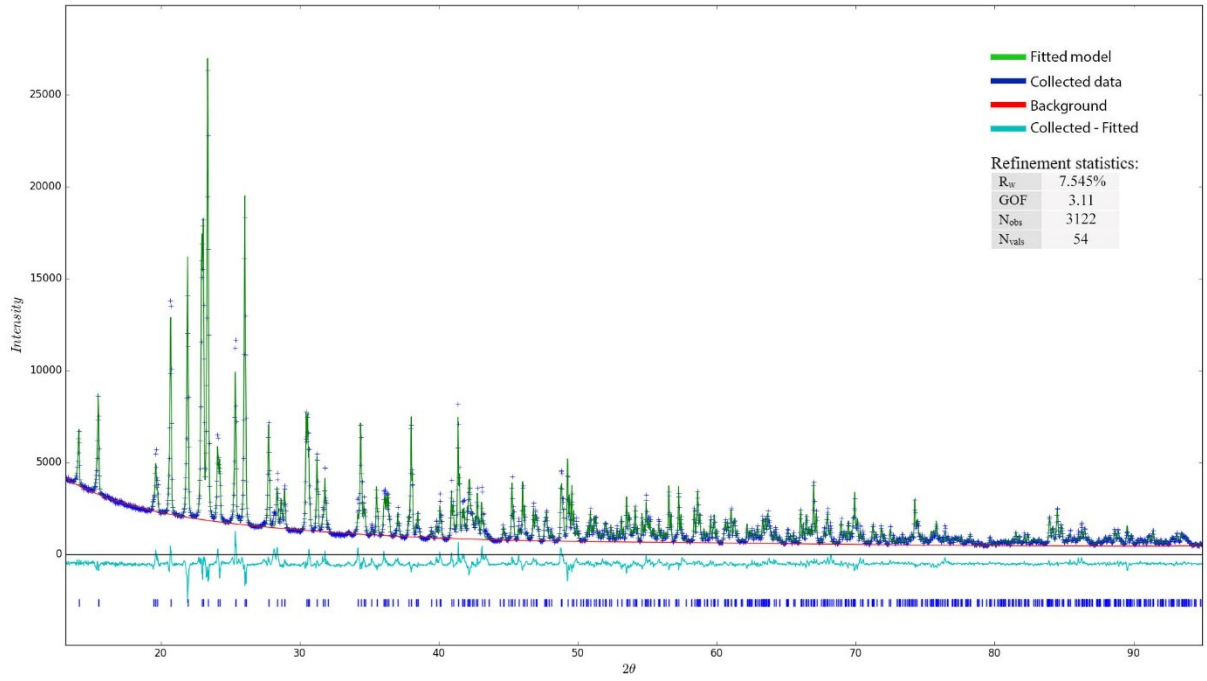

Figure S5 – Rietveld-refined fit of the $Al_2W_3O_{12}$ structural model to XRD data.

Table S1 – Atomic parameters of M sites (occupied by Mo or W) of $Al_2Mo_3O_{12}$ and $Al_2W_3O_{12}$ and the fractional occupancy (SOF) of Mo and W on the occupied sites extracted from Rietveld refined models to Cu Kα XRD data.

site	x	y	z	SOF Mo	SOF W
$Al_2Mo_3O_{12}$					
M1	-0.0055(10)	0.2321(11)	0.4874(7)	1	0
M2	0.3534(9)	0.1150(15)	0.1285(7	1	0

			)		
M3	0.1404(8)	0.1087(13)	0.2512(6)	1	0
M4	0.1496(9)	0.6207(15)	0.3794(7)	1	0
M5	0.3525(8)	0.6297(13)	0.2160(6)	1	0
M6	0.0097(10)	0.7487(14)	0.0231(7)	1	0
$Al_2W_3O_{12}$					
M1	0.25000	0.00000	0.4746(4)	0	1
M2	0.11719(30)	0.35596(25)	0.3956(3)	0	1

Electrochemistry

Table S2 - Measured long-term cycle discharge capacities for the 1st, 2nd, 25th, 50th and 100th cycle against lithium at 30 mAh/g for the solid solutions of $Al_2W_xMo_{3-x}O_{12}$

	Discharge Capacity (mAh/g)					Charge Capacity (mAh/g)				
Cycle	**1st**	**2nd**	**25th**	**50th**	**100th**	**1st**	**2nd**	**25th**	**50th**	**100th**
$Al_2Mo_3O_{12}$	883	415	168	151	136	421	351	166	149	135
$Al_2W_{0.5}Mo_{2.5}O_{12}$	829	426	216	184	173	423	384	208	183	172
$Al_2W_1MoO_{12}$	854	349	129	120	112	359	300	127	120	112
$Al_2W_{1.5}Mo_{1.5}O_{12}$	832	340	124	105	87	353	280	122	102	85
$Al_2W_2Mo_1O_{12}$	788	291	155	130	114	302	276	152	125	113
$Al_2W_{2.5}Mo_{0.5}O_{12}$	651	238	114	95	90	245	213	112	95	89
$Al_2W_3O_{12}$	654	228	119	101	96	230	211	117	100	95

Table S3 - Long-term cycle discharge capacities for the 1st, 2nd, 25th, 50th and 100th cycle against Na at 25 mAh/g for the solid solutions of $Al_2W_xMo_{3-x}O_{12}$

	Discharge Capacity (mAh/g)					Charge Capacity (mAh/g)				
Cycle	**1st**	**2nd**	**25th**	**50th**	**100th**	**1st**	**2nd**	**25th**	**50th**	**100th**
$Al_2Mo_3O_{12}$	154	51	36	33	28	33	33	34	33	28
$Al_2W_{0.5}Mo_{2.5}O_{12}$	180	50	31	29	28	26	26	29	28	27
$Al_2W_1MoO_{12}$	111	43	27	25	23	20	21	24	24	23
$Al_2W_{1.5}Mo_{1.5}O_{12}$	74	24	17	18	19	14	13	15	17	18
$Al_2W_2Mo_1O_{12}$	93	24	16	16	16	16	16	15	15	15
$Al_2W_{2.5}Mo_{0.5}O_{12}$	84	20	13	12	12	14	13	12	12	11
$Al_2W_3O_{12}$	42	16	12	12	13	11	11	11	12	13

Differential capacity plots

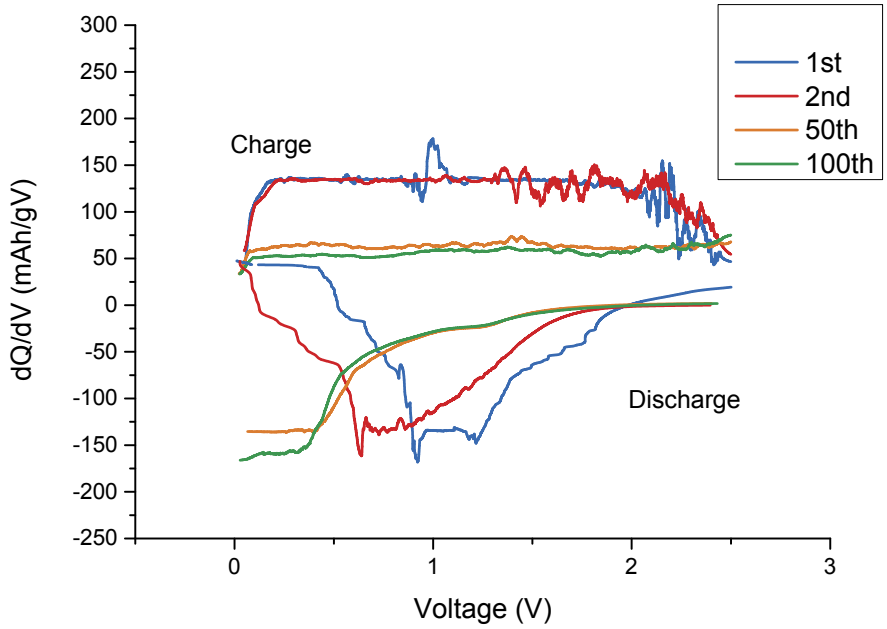

Figure S6 – Differential capacity plots of $Al_2Mo_3O_{12}$ illustrating the significant changes observed between the 1st and 100th cycles.

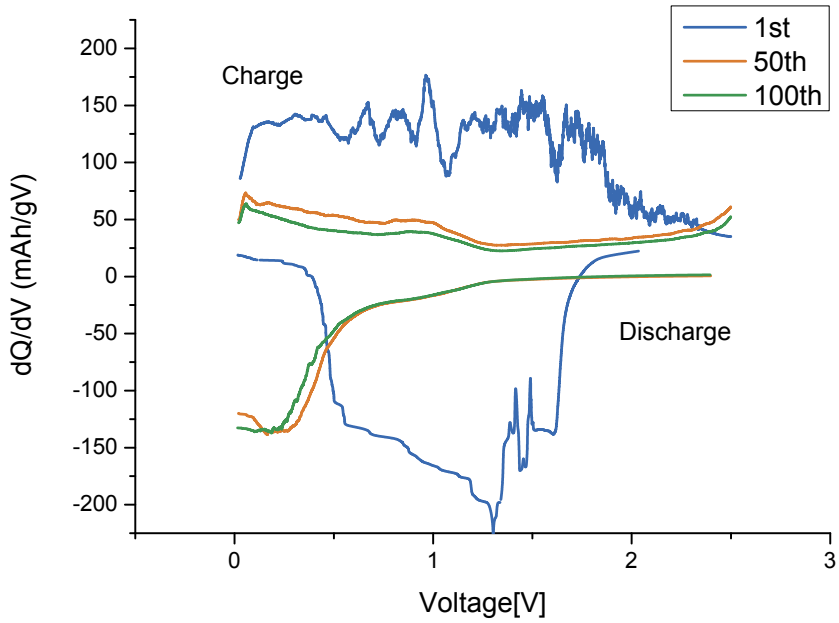

Figure S7 – Differential capacity plots of $Al_2Mo_{1.5}W_{1.5}O_{12}$ illustrating the significant changes observed between the 1st and 100th cycles, similar to Figure S6.

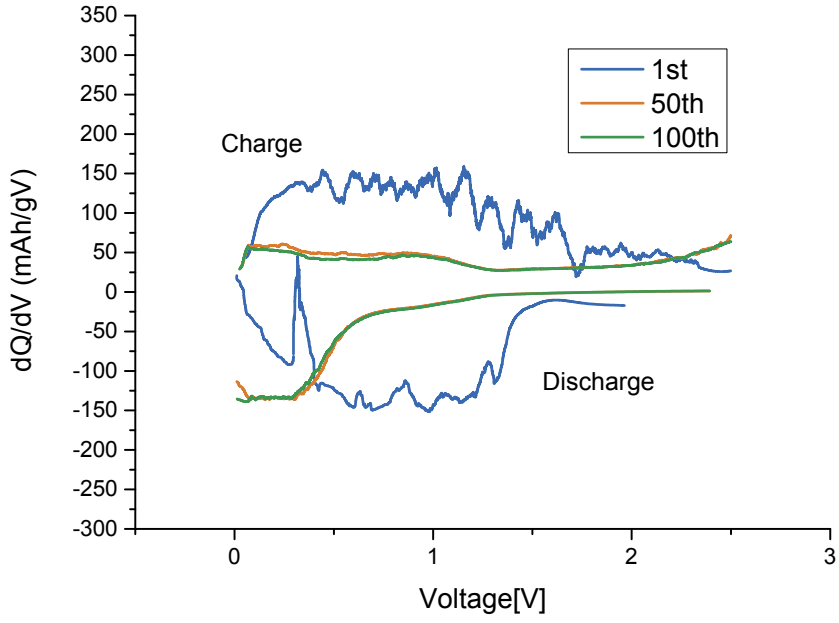

Figure S8 – Differential capacity plots of $Al_2W_3O_{12}$ illustrating the significant changes observed between the 1st and 100th cycles, similar to Figure S7 and S8.

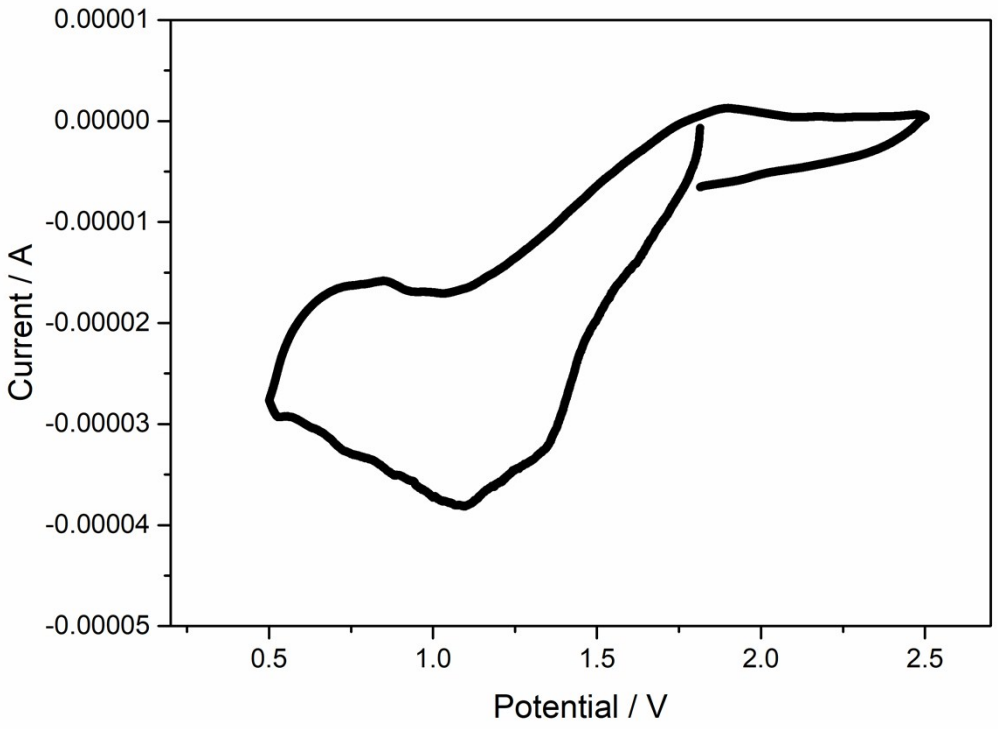

Figure S9 – CV curve during the first cycle of the $Al_2Mo_3O_{12}$ electrode in a custom-made cell. The oxidation feature at 1.2 V and reduction features at 0.75 and 1.8 V can be seen in the data.