Electronic Supplementary Material for CrystEngComm
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Supporting Information

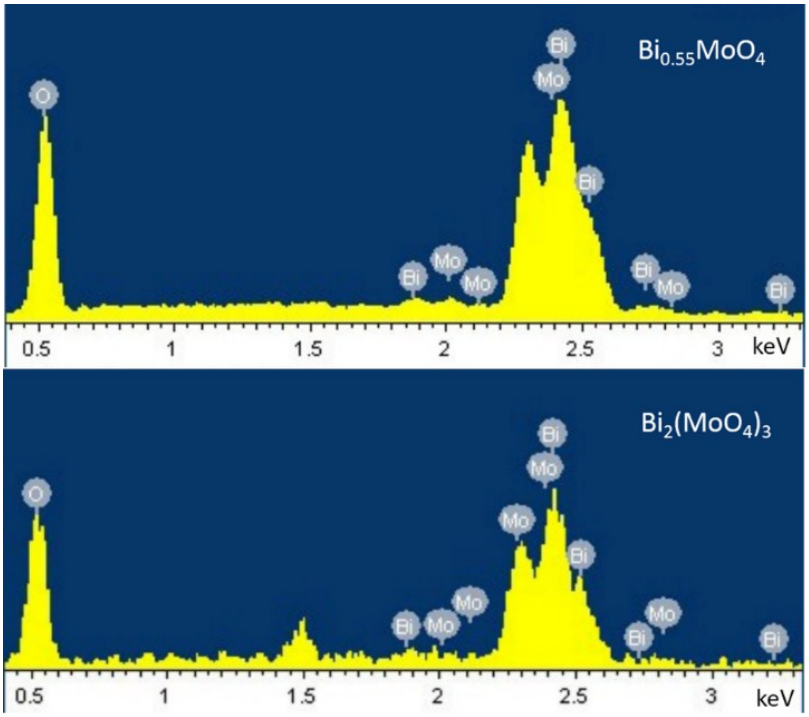

Fig. S1 EDS spectra of (top) $Bi_{0.55}MoO_4$ and (bottom) $Bi_2(MoO_4)_3$.

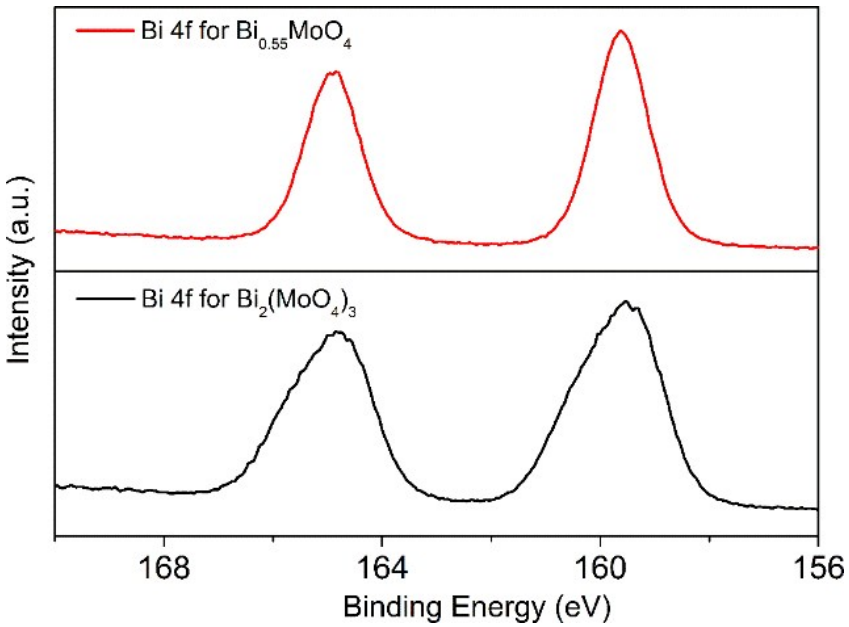

Fig. S2 Bi 4f XPS spectra of $Bi_{0.55}MoO_4$ and $Bi_2(MoO_4)_3$.

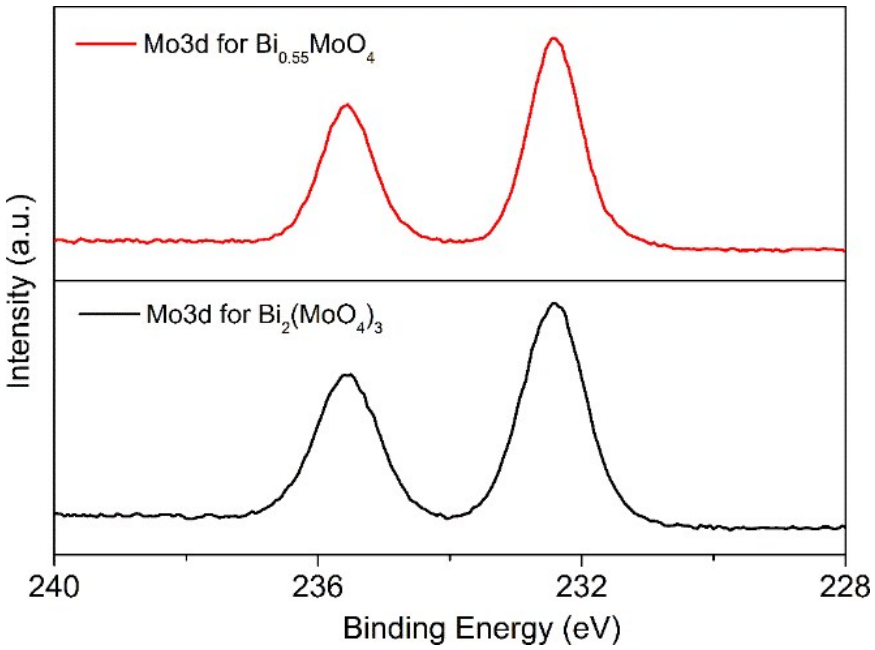

Fig. S3 Mo 3d XPS spectra of $Bi_{0.55}MoO_4$ and $Bi_2(MoO_4)_3$.

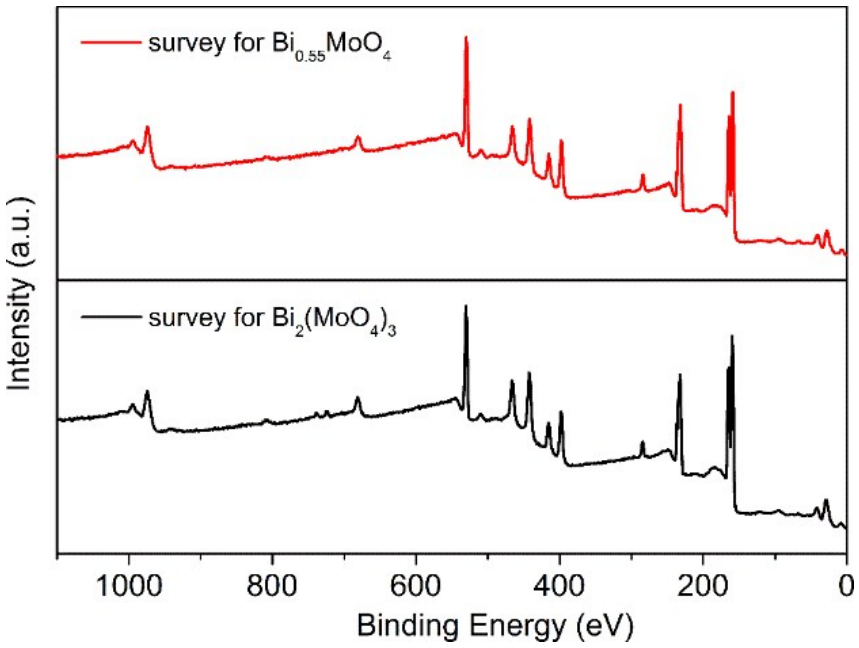

Fig. S4 XPS survey spectra of $Bi_{0.55}MoO_4$ and $Bi_2(MoO_4)_3$.

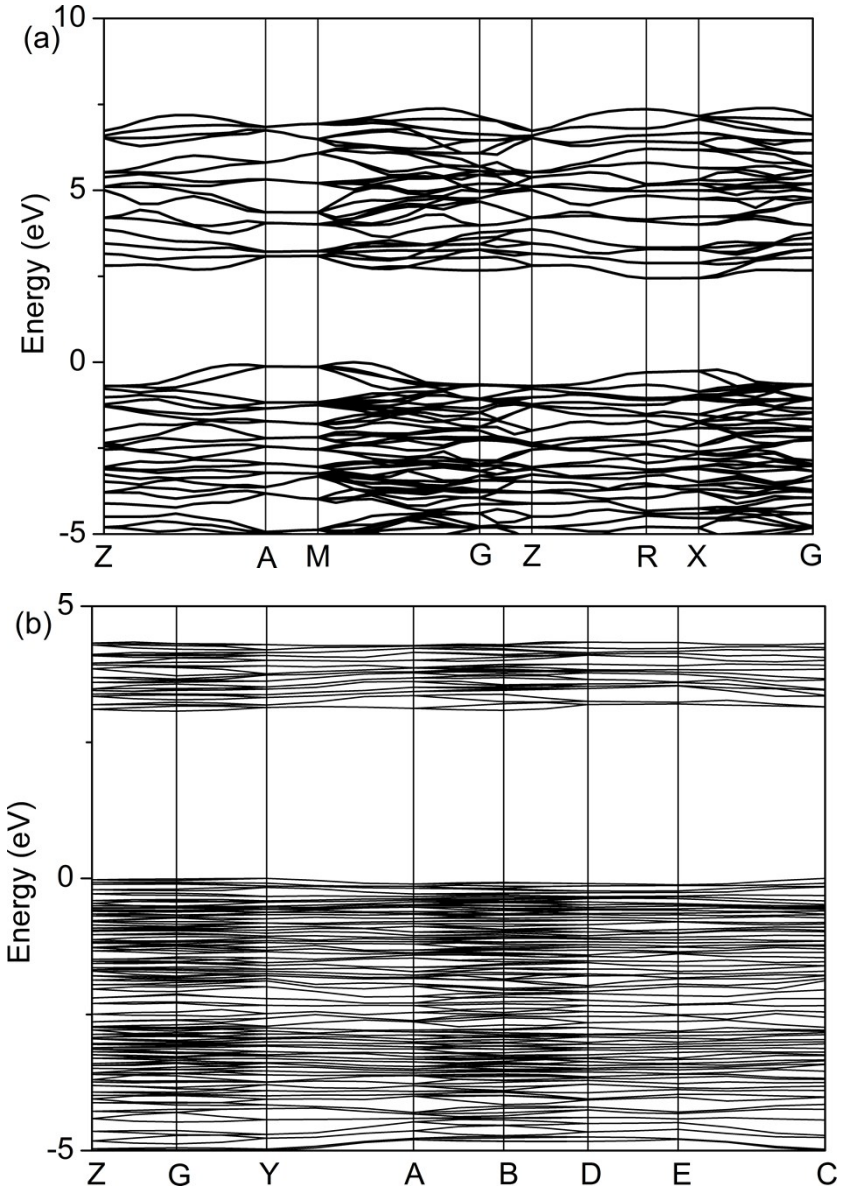

Fig. S5 The band structures of (a) $Bi_{0.55}MoO_4$ and (b) $Bi_2(MoO_4)_3$ along high symmetry points in the first Brilluoin zone.

Table S1 The atomic coordinates and their equivalent isotropic thermal parameters for $Bi_{0.55}MoO_4$

	x	y	z	$U_{eq}(Å^2)$	Site
Bi1	0.50000	0.25000	0.87500	0.015	4b
Mo1	0.00000	0.75000	0.87500	0.012	4a
O1	0.24150	0.59880	0.95810	0.023	16f

Table S2 The atomic coordinates and their equivalent isotropic thermal parameters for $Bi_2(MoO_4)_3$

	x	y	z	$U_{eq}(Å^2)$	Site
Bi1	0.99586	0.36209	0.75579	0.014	4e

Bi2	0.67580	0.37011	0.08372	0.015	4e
Mo2	0.68741	0.15135	0.60944	0.014	4e
Mo1	0.88419	0.38886	0.41660	0.014	4e
Mo3	0.46143	0.36686	0.69562	0.015	4e
O1	0.69260	0.31550	0.69830	0.020	4e
O2	0.24450	0.29080	0.69790	0.016	4e
O3	0.71170	0.30050	0.43450	0.020	4e
O4	0.93420	0.19580	0.65260	0.016	4e
O5	0.67960	0.05260	0.72270	0.022	4e
O6	0.95580	0.44920	0.58110	0.015	4e
O7	0.81960	0.44650	0.25610	0.016	4e
O8	1.05390	0.29210	0.41310	0.021	4e
O9	0.49610	0.44070	0.83470	0.022	4e
O10	0.45050	0.20610	0.57230	0.021	4e
O11	0.69350	0.06380	0.48110	0.021	4e
O12	0.39350	0.46900	0.58490	0.026	4e

Table S3 Interatomic distances (Å) in $Bi_{0.55}MoO_4$

Bi1-O1	2.469(3)	Bi1-O1	2.487(3)	Mo1-O1	1.776(3)
Bi1-O1	2.469(3)	Bi1-O1	2.487(3)	Mo1-O1	1.776(3)
Bi1-O1	2.469(3)	Bi1-O1	2.487(3)	Mo1-O1	1.776(3)
Bi1-O1	2.469(3)	Bi1-O1	2.487(3)	Mo1-O1	1.776(3)

Table S4 Interatomic distances (Å) in $Bi_2(MoO_4)_3$

Bi1-O6	2.145(4)	Bi1-O5	2.617(4)	Bi2-O7	2.167(4)	Bi2-O11	2.616(4)
Bi1-O4	2.226(4)	Bi1-O7	2.643(4)	Bi2-O2	2.240(4)	Bi2-O8	2.673(4)
Bi1-O2	2.311(4)	Bi1-O11	2.751(4)	Bi2-O4	2.302(4)	Bi2-O10	2.324(4)
Bi1-O1	2.341(4)	Bi1-O7	2.167(4)	Bi2-O10	2.324(4)	Bi2-O11	2.616(4)
Mo1-O3	1.732(4)	Mo2-O5	1.707(4)	Mo3-O12	1.696(5)		
Mo1-O8	1.726(4)	Mo2-O11	1.756(4)	Mo3-O9	1.730(4)		
Mo1-O7	1.861(4)	Mo2-O10	1.886(4)	Mo3-O1	1.873(4)		
Mo1-O6	1.915(4)	Mo2-O4	1.922(4)	Mo3-O2	1.894(4)		
Mo1-O6	2.233 (4)	Mo2-O1	2.128(4)	Mo3-O10	2.293(5)		