Electronic Supplementary Information

$ScMO(BO_3)$ (M = Ca, Cd)：New Sc-based oxyborates featuring interesting edge-sharing sandwich-like chains and UV cut-off edges

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Table S1 Bond lengths [Å] and angles [deg] for (a) $ScCaO(BO_3)$ and (b) $ScCdO(BO_3)$.

(a) $ScCaO(BO_3)$

Sc(1)-O(1)#1	2.0806(12)	O(1)-Sc(1)-O(3)#1	170.91(6)
Sc(1)-O(1)	2.0806(12)	O(1)#2-Sc(1)-O(3)#1	90.49(6)
Sc(1)-O(1)#2	2.0869(18)	O(2)-Sc(1)-O(3)#1	81.39(6)
Sc(1)-O(2)	2.1502(19)	O(3)-Sc(1)-O(3)#1	96.91(8)
Sc(1)-O(3)	2.2472(13)	O(1)-Ca(1)-O(4)	82.41(6)
Sc(1)-O(3)#1	2.2472(13)	O(1)-Ca(1)-O(4)#1	82.41(6)
Ca(1)-O(1)	2.3035(19)	O(4)-Ca(1)-O(4)#1	93.44(8)
Ca(1)-O(4)	2.3101(15)	O(1)-Ca(1)-O(2)#7	89.11(5)
Ca(1)-O(4)#1	2.3101(15)	O(4)-Ca(1)-O(2)#7	170.91(7)
Ca(1)-O(2)#7	2.4215(15)	O(4)#1-Ca(1)-O(2)#7	88.64(5)
Ca(1)-O(2)#8	2.4215(14)	O(1)-Ca(1)-O(2)#8	89.11(5)
Ca(1)-O(3)#7	2.4298(19)	O(4)-Ca(1)-O(2)#8	88.64(5)
Ca(1)-O(4)#9	2.696(2)	O(4)#1-Ca(1)-O(2)#8	170.91(7)
B(1)-O(4)#1	1.373(3)	O(2)#7-Ca(1)-O(2)#8	87.98(7)
B(1)-O(3)#11	1.381(3)	O(1)-Ca(1)-O(3)#7	154.04(6)
B(1)-O(2)	1.383(3)	O(4)-Ca(1)-O(3)#7	114.41(6)
O(1)#1-Sc(1)-O(1)	107.86(8)	O(4)#1-Ca(1)-O(3)#7	114.41(6)
O(1)#1-Sc(1)-O(1)#2	82.76(6)	O(2)#7-Ca(1)-O(3)#7	72.49(5)
O(1)-Sc(1)-O(1)#2	82.76(6)	O(2)#8-Ca(1)-O(3)#7	72.49(5)
O(1)#1-Sc(1)-O(2)	104.21(6)	O(1)-Ca(1)-O(4)#9	151.42(7)
O(1)-Sc(1)-O(2)	104.21(6)	O(4)-Ca(1)-O(4)#9	78.12(6)
O(1)#2-Sc(1)-O(2)	167.71(7)	O(4)#1-Ca(1)-O(4)#9	78.12(6)
O(1)#1-Sc(1)-O(3)	170.91(6)	O(2)#7-Ca(1)-O(4)#9	110.96(5)
O(1)-Sc(1)-O(3)	77.15(6)	O(2)#8-Ca(1)-O(4)#9	110.96(5)
O(1)#2-Sc(1)-O(3)	90.49(6)	O(3)#7-Ca(1)-O(4)#9	54.54(6)
O(2)-Sc(1)-O(3)	81.39(6)	O(4)#1-B(1)-O(3)#11	118.0(2)
O(1)#1-Sc(1)-O(3)#1	77.15(6)	O(4)#1-B(1)-O(2)	121.0(2)
O(3)#11-B(1)-O(2)	121.1(2)		

Symmetry transformations used to generate equivalent atom
#1 x,y+1,z #2 -x+1,-y+2,-z+1 #3 -x+1,-y+3,-z+1

#4 x,y-1,z #5 x-1/2,y,-z+3/2 #6 x-1/2,y+1,-z+3/2

#7 x+1/2,y,-z+3/2 #8 x+1/2,y-1,-z+3/2 #9 -x+1,-y+1,-z+2

#10 -x+1,-y+2,-z+2 #11 -x+1/2,-y+2,z+1/2 #12 -x+1/2,-y+2,z-1/2

(b) $ScCdO(BO_3)$

Cd(1)/Sc(1)-O(1)#1	2.181(6)	O(2)#3-Cd(1)/Sc(1)-O(3)#3	77.0(2)
Cd(1)/Sc(1)-O(4)	2.208(5)	O(1)#1-Cd(1)/Sc(1)-O(3)#4	88.23(19)
Cd(1)/Sc(1)-O(4)#2	2.208(5)	O(4)-Cd(1)/Sc(1)-O(3)#4	84.9(2)
Cd(1)/Sc(1)-O(2)#3	2.252(6)	O(4)#2-Cd(1)/Sc(1)-O(3)#4	172.7(3)
Cd(1)/Sc(1)-O(3)#3	2.382(5)	O(2)#3-Cd(1)/Sc(1)-O(3)#4	77.0(2)
Cd(1)/Sc(1)-O(3)#4	2.382(5)	O(3)#3-Cd(1)/Sc(1)-O(3)#4	90.1(2)
Cd(2)/Sc(2)-O(1)	2.091(6)	O(1)-Cd(2)/Sc(2)-O(1)#1	82.0(2)
Cd(2)/Sc(2)-O(1)#1	2.097(4)	O(1)-Cd(2)/Sc(2)-O(1)#6	82.0(2)
Cd(2)/Sc(2)-O(1)#6	2.097(4)	O(1)#1-Cd(2)/Sc(2)-O(1)#6	107.0(3)
Cd(2)/Sc(2)-O(3)	2.153(7)	O(1)-Cd(2)/Sc(2)-O(3)	169.7(3)
Cd(2)/Sc(2)-O(2)	2.290(5)	O(1)#1-Cd(2)/Sc(2)-O(3)	103.9(2)
Cd(2)/Sc(2)-O(2)#2	2.290(5)	O(1)#6-Cd(2)/Sc(2)-O(3)	103.9(2)
B(1)-O(2)#10	1.349(12)	O(1)-Cd(2)/Sc(2)-O(2)	92.1(2)
B(1)-O(3)	1.394(12)	O(1)#1-Cd(2)/Sc(2)-O(2)	171.0(2)
B(1)-O(4)	1.363(12)	O(1)#6-Cd(2)/Sc(2)-O(2)	78.68(19)
O(1)#1-Cd(1)/Sc(1)-O(4)	86.3(3)	O(3)-Cd(2)/Sc(2)-O(2)	80.9(2)
O(1)#1-Cd(1)/Sc(1)-O(4)#2	86.3(3)	O(1)-Cd(2)/Sc(2)-O(2)#2	92.1(2)
O(4)-Cd(1)/Sc(1)-O(4)#2	99.5(3)	O(1)#1-Cd(2)/Sc(2)-O(2)#2	78.68(19)
O(1)#1-Cd(1)/Sc(1)-O(2)#3	158.9(2)	O(1)#6-Cd(2)/Sc(2)-O(2)#2	171.0(2)
O(4)-Cd(1)/Sc(1)-O(2)#3	106.9(3)	O(3)-Cd(2)/Sc(2)-O(2)#2	80.9(2)
O(4)#2-Cd(1)/Sc(1)-O(2)#3	106.9(3)	O(2)-Cd(2)/Sc(2)-O(2)#2	94.8(3)
O(1)#1-Cd(1)/Sc(1)-O(3)#3	88.23(19)	O(2)#10-B(1)-O(4)	119.7(9)
O(4)-Cd(1)/Sc(1)-O(3)#3	172.7(3)	O(2)#10-B(1)-O(3)	121.5(8)
O(4)#2-Cd(1)/Sc(1)-O(3)#3	84.9(2)	O(4)-B(1)-O(3)	118.8(9)

Symmetry transformations used to generate equivalent atom

#1 -x+2,-y+2,-z+2 #2 x,y+1,z #3 x+1/2,y+1,-z+3/2

#4 x+1/2,y,-z+3/2 #5 x,y-1,z #6 -x+2,-y+1,-z+2

#7 x-1/2,y-1,-z+3/2 #8 x-1/2,y,-z+3/2 #9 -x+3/2,-y+1,z+1/2

#10 -x+3/2,-y+1,z-1/2

Table S2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacementparameters ($Å^2 \times 10^3$) for $ScCaO(BO_3)$**.** U(eq) is defined as one third of the trace of theorthogonalized U_{ij} tensor, and calculated bond valence sum (BVS)

	x/*a*	y/*b*	z/*c*	U(eq)	BVS
Sc(1)	3899(1)	12500	5716(1)	8(1)	2.933
Ca(1)	5887(1)	7500	8409(1)	8(1)	2.064
B(1)	3046(3)	12500	8649(3)	8(1)	2.936
O(1)	5020(2)	7500	6157(2)	8(1)	1.987
O(2)	2435(2)	12500	7343(2)	10(1)	1.994
O(3)	2663(2)	7500	4892(2)	10(1)	1.938
O(4)	4379(2)	2500	8748(2)	16(1)	1.786

Table S3 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacementparameters ($Å^2 \times 10^3$) for $ScCdO(BO_3)$**.** U(eq) is defined as one third of the trace of theorthogonalized U_{ij} tensor.

	x/a	y/b	z/c	S.O.F	U(eq)
Cd(1)	10909(1)	12500	6730(1)	0.741	11(1)
Sc(1)	10909(1)	12500	6730(1)	0.259	11(1)
Cd(2)	8864(1)	7500	9240(1)	0.259	14(1)
Sc(2)	8864(1)	7500	9240(1)	0.741	14(1)
B(1)	8161(10)	7500	6250(11)	1	14(2)
O(1)	9934(6)	7500	11142(6)	1	14(1)
O(2)	7476(7)	2500	9991(7)	1	23(2)
O(3)	7447(7)	7500	7517(7)	1	21(2)
O(4)	9534(7)	7500	6293(10)	1	41(2)

Table S4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for (a) $ScCaO(BO_3)$ and (b) $ScCdO(BO_3)$

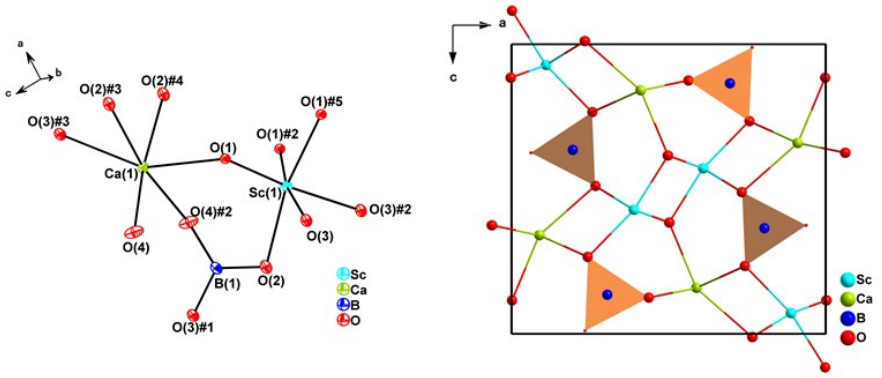
(a) $ScCaO(BO_3)$

	U11	U22	U33	U23	U13	U12
Ca(1)	7(1)	8(1)	9(1)	0	-1(1)	0
Sc(1)	7(1)	8(1)	9(1)	0	2(1)	0
B(1)	11(1)	6(1)	7(1)	0	2(1)	0
O(1)	6(1)	11(1)	6(1)	0	0(1)	0
O(2)	13(1)	12(1)	7(1)	0	0(1)	0
O(3)	11(1)	14(1)	6(1)	0	-0(1)	0
O(4)	8(1)	10(1)	28(1)	0	4(1)	0

(b) $ScCdO(BO_3)$

	U11	U22	U33	U23	U13	U12
Cd(1)	11(1)	9(1)	14(1)	0	5(1)	0
Cd(2)	13(1)	11(1)	19(1)	0	-4(1)	0
Sc(1)	11(1)	9(1)	14(1)	0	5(1)	0
Sc(2)	13(1)	11(1)	19(1)	0	-4(1)	0
B(1)	14(5)	17(5)	11(5)	0	-3(4)	0
O(1)	12(3)	20(3)	11(3)	0	1(2)	0
O(2)	17(3)	47(5)	5(3)	0	-4(2)	0
O(3)	23(3)	29(4)	12(3)	0	-6(3)	0
O(4)	11(3)	28(4)	84(7)	0	-8(4)	0

Figure S1 The unit cell and asymmetric unit of $ScCaO(BO_3)$



Asymmetric unit of selected symmetry-equivalent atoms in$ScCaO(BO_3)$, showing the linkages and coordination spheres with 50 % thermal ellipsoids and atom labels. Symmetry codes:(#1) 0.5-x, 2-y, 0.5+z; (#2) x, 1+y, z; (#3) 0.5+x, 1.5-y, 1.5-z; (#4) 0.5+x, 2.5-y, 1.5-z; (#5) 1-x, 0.5+y, 1-z.

Figure S2 Crystal structure of $ScCdO(BO_3)$

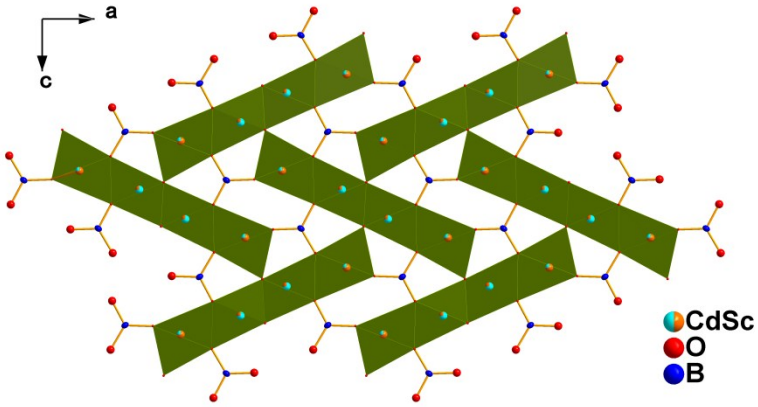
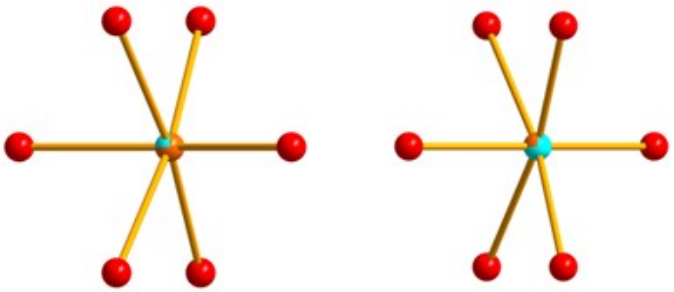
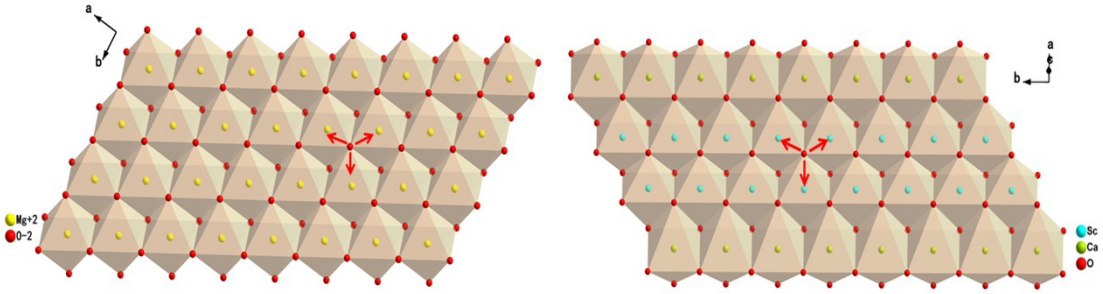


Figure S3 The coordination environments of cations in $ScCdO(BO_3)$.



$Sc(1)/Cd(1)O_6$ **$Sc(2)/Cd(2)O_6$**

Figure S4 Comparison of the mode of octahedral connection between (a) talcum and (b) $ScCaO(BO_3)$.



(a) **(b)**

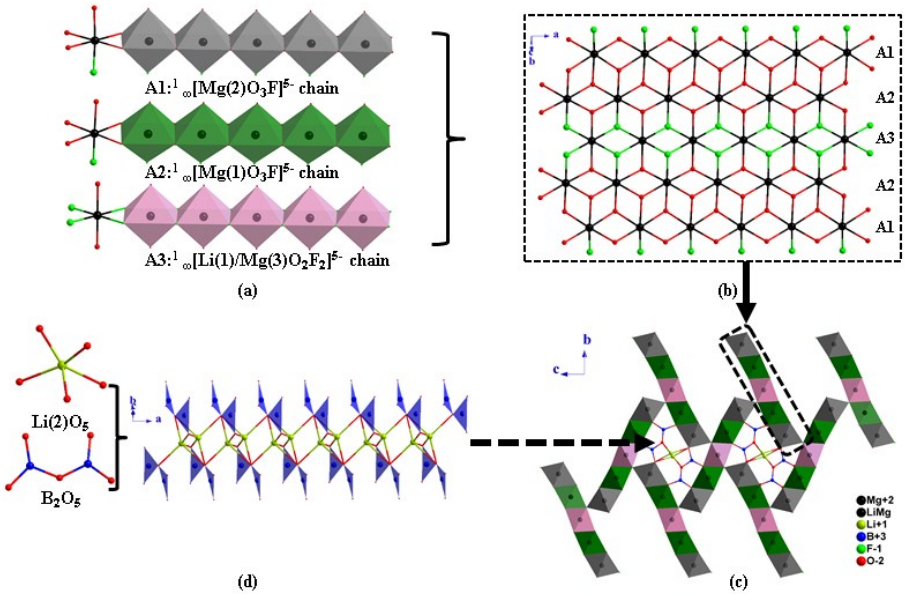
(a)The octahedral layer in talcum. (b) The octahedral chain in $ScCaO(BO_3)$

The connection mode of octahedra of $ScMO(BO_3)$(M =Ca and Cd) is similar to that of talcum.[1] Viewing from Figure S4a, the Mg atoms are bonded to six oxygen atoms to form $[MgO_6]$ octahedra, which connect with each other by edge-sharing to form the 2D layer in the *ab* plane. Similarly, in Figure S4b, an infinite 1D chain is composed by $[CaO_6]$ octahedra by sharing O-O edges along the *b* axis.

Reference

[1] S. B. Hendricks, M. E. Jefferson, *Am. Mineral.*, 1938, **25**, 851.

Figure S5 The crystal structure of $Li_{0.8}Mg_{2.1}B_2O_5F$.



(a) The coordination of Mg(1), Mg(2) and Li(1)/Mg(3); A2, A1, A3 chains composed of $^1_\infty[Mg(1)O_3F]^{5-}$, $^1_\infty[Mg(2)O_3F]^{5-}$ and $^1_\infty[Li(1)/Mg(3)O_2F_2]^{5-}$ by edge-sharing. (b) BBU. (c) Crystal structure of $Li_{0.8}Mg_{2.1}B_2O_5F$ projected along the *a* axis. (d) Zigzag chain composed of isolated B_2O_5 blocks and $Li(2)O_5$.

Figure S6 The infrared spectra of (a) $ScCaO(BO_3)$ and (b) $ScCdO(BO_3)$.

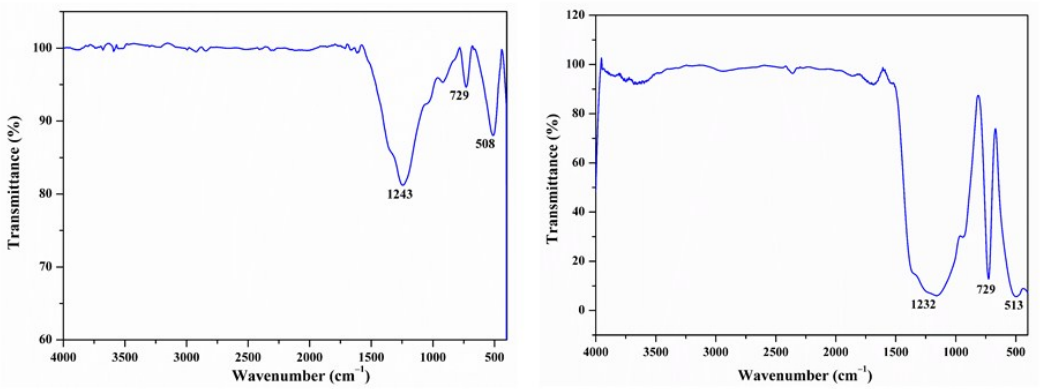
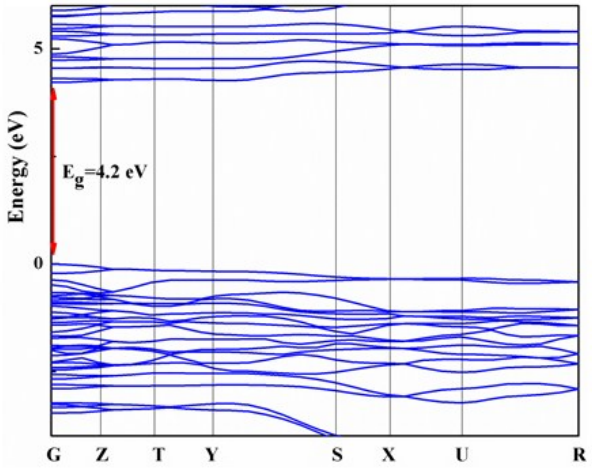


Figure S7 Band structure of $ScCaO(BO_3)$.



(a)

Figure S8 Birefringence of $ScCaO(BO_3)$.