Electronic Supplementary Information

From $BaAl_2(BO_3)_2O$ to $SnAl_2(BO_3)_2F_2$: Structure Transformation Based on the Ions Regulation

Ya Wang,[†a,b] Jian Han,[†a,b] Junben Huang,[a] Zhihua Yang,[a,b] Shuzhao Huang[a] and Shilie Pan[*a,b]

[a] CAS Key Laboratory of Functional Materials and Devices for Special Environments; Xinjiang Technical Institute of Physics & Chemistry, CAS; Xinjiang Key Laboratory of Electronic Information Materials and Devices, 40-1 South Beijing Road, Urumqi 830011, China.

[b] Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China.

* Corresponding author: slpan@ms.xjb.ac.cn.

† These authors contributed equally to this work.

Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters (U_{eq}, $Å^2 \times 10^3$), and bond valence sums (BVS) of each atom for $SnAl_2(BO_3)_2F_2$.

Atom	**x**	**y**	**z**	**U_{eq}**	**BVS**
Sn(1)	0	2500	9(1)	9(1)	1.954
Al(1)	1230(2)	0	5000	6(1)	3.115
B(1)	0	848(7)	2750(8)	6(2)	3.057
O(1)	0	134(4)	3798(5)	7(1)	2.001
O(2)	955(3)	1278(3)	2194(4)	8(1)	2.088
F(1)	2295(2)	-205(2)	6250	8(1)	0.969

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Bond lengths (Å) and angles (°) for $SnAl_2(BO_3)_2F_2$.

Sn(1)-O(2)#1	2.249(4)	F(1)-Al(1)-F(1)#4	91.94(19)
Sn(1)-O(2)#2	2.249(4)	F(1)-Al(1)-O(2)#5	89.47(15)
Sn(1)-O(2)#3	2.249(4)	F(1)#4-Al(1)-O(2)#5	90.93(15)
Sn(1)-O(2)	2.249(4)	F(1)-Al(1)-O(2)#6	90.93(15)
Al(1)-F(1)	1.812(2)	F(1)#4-Al(1)-O(2)#6	89.47(15)
Al(1)-F(1)#4	1.812(2)	O(2)#5-Al(1)-O(2)#6	179.4(2)
Al(1)-O(2)#5	1.854(4)	F(1)-Al(1)-O(1)	174.03(18)
Al(1)-O(2)#6	1.854(4)	F(1)#4-Al(1)-O(1)	93.61(14)
Al(1)-O(1)	1.912(4)	O(2)#5-Al(1)-O(1)	88.24(19)
Al(1)-O(1)#7	1.912(4)	O(2)#6-Al(1)-O(1)	91.3(2)
B(1)-O(2)#1	1.363(6)	F(1)-Al(1)-O(1)#7	93.61(14)
B(1)-O(2)	1.363(6)	F(1)#4-Al(1)-O(1)#7	174.03(18)
B(1)-O(1)	1.366(9)	O(2)#5-Al(1)-O(1)#7	91.3(2)
O(2)#1-Sn(1)-O(2)	79.99(18)	O(2)#6-Al(1)-O(1)#7	88.24(19)
O(2)#1-Sn(1)-O(2)	109.3(2)	O(1)-Al(1)-O(1)#7	80.9(2)
O(2)#1-Sn(1)-O(2)#2	109.3(2)	O(2)#1-B(1)-O(1)	124.0(3)
O(2)#1-Sn(1)-O(2)#3	79.99(18)	O(2)-B(1)-O(1)	124.0(3)
O(2)#1-Sn(1)-O(2)#3	60.28(18)	O(2)#1-B(1)-O(2)	111.9(7)
O(2)#1-Sn(1)-O(2)	60.28(18)		

Symmetry transformations used to generate equivalent atoms:

#1 -x, y, z; #2 x, -y+1/2, z; #3 -x+0, -y+1/2, z;

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

#7 -x, -y, -z+1

Table S3. The basic information of tin (Ⅱ) borates.

Compounds	Space group	B-O groups	A/B
$SnB_8O_{11}(OH)_4$	$P2_1/n$	$[B_8O_{11}(OH)_4]_\infty$ layer	0.13
β-SnB_4O_7	$Pmn2_1$	3D network	0.25
$Sn_2B_7O_{12}F$	$C2/c$	$[B_7O_{12}]_\infty$ layer	0.28
$Sn_2B_5O_9Cl$	$Pnn2$	3D network	0.4
$SnB_2O_3F_2$	$P3_1m$	$[B_2O_3F_2]_\infty$ layer	0.5
$Sn_2B_3O_6(OH)$	$P2_1/n$	$[B_3O_6(OH)]_\infty$ chain	0.67
$Sn_3B_4O_9$	$P2_1/c$	$[B_4O_9]_\infty$ layer	0.75
$Sn_3[B_3O_7]F$	$Pna2_1$	Isolated B_3O_7	1
$Sn_3[B_3O_7]I$	$Pbca$	$[B_3O_7]_\infty$ chain	1
$SnAl_2(BO_3)_2F_2$	***$I4_1/amd$***	**Isolated BO_3**	**1.5**

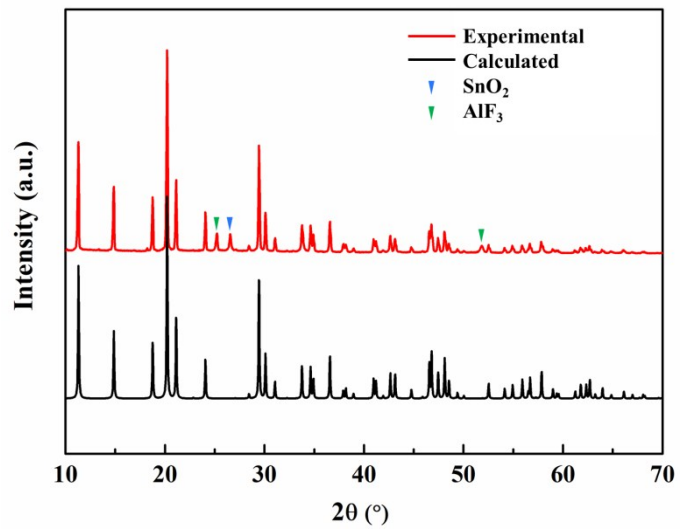

Fig. S1 The experimental and calculated XRD patterns of $SnAl_2(BO_3)_2F_2$.

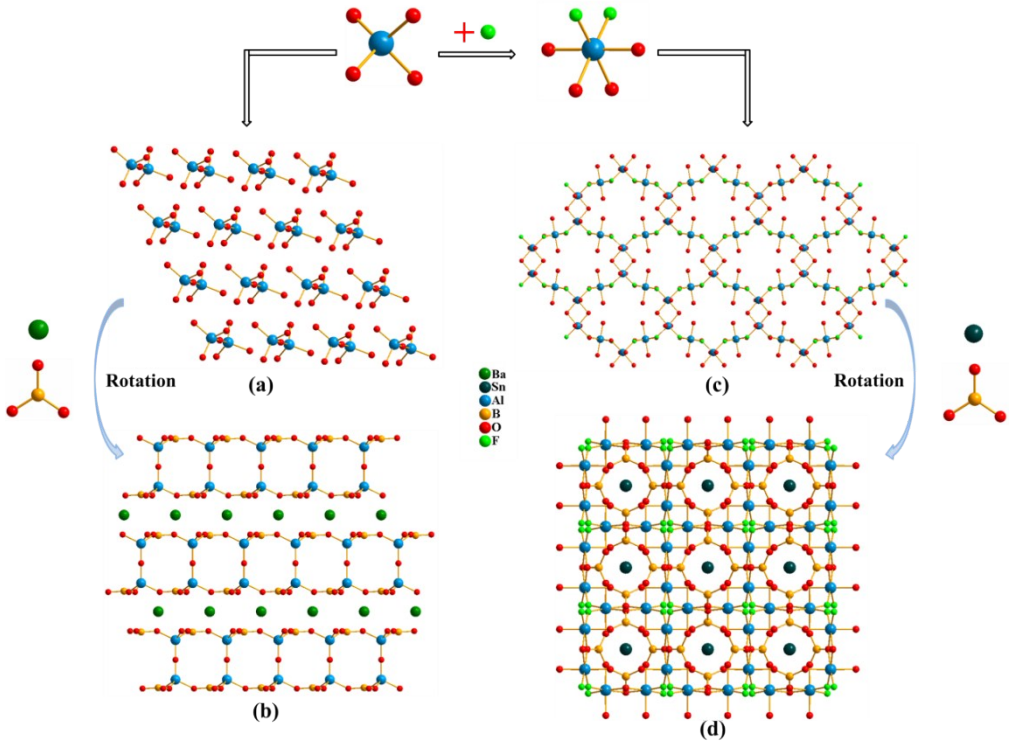

Fig. S2 (a, b) Al-O groups and holistic structure of $BaAl_2(BO_3)_2O$; (c, d) Al-O-F framework and holistic structure of $SnAl_2(BO_3)_2F_2$.

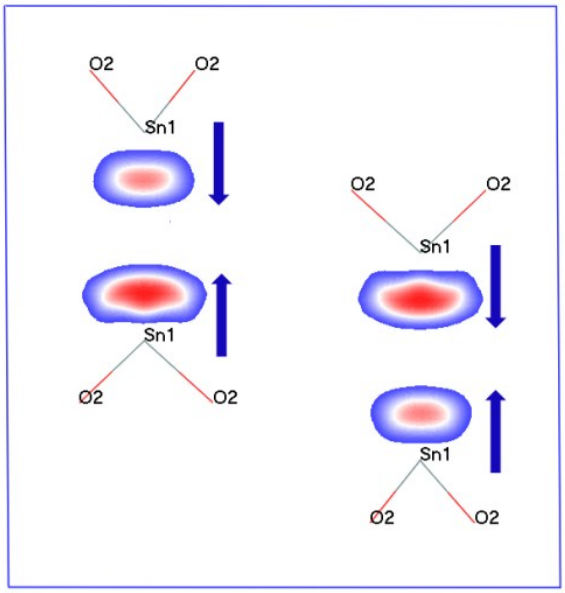

Fig. S3 The electron localization function of $SnAl_2(BO_3)_2F_2$.