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Supporting Information for "*Design of ternary alkaline-earth metal Sn(II) oxides with potential good p-type conductivity*"

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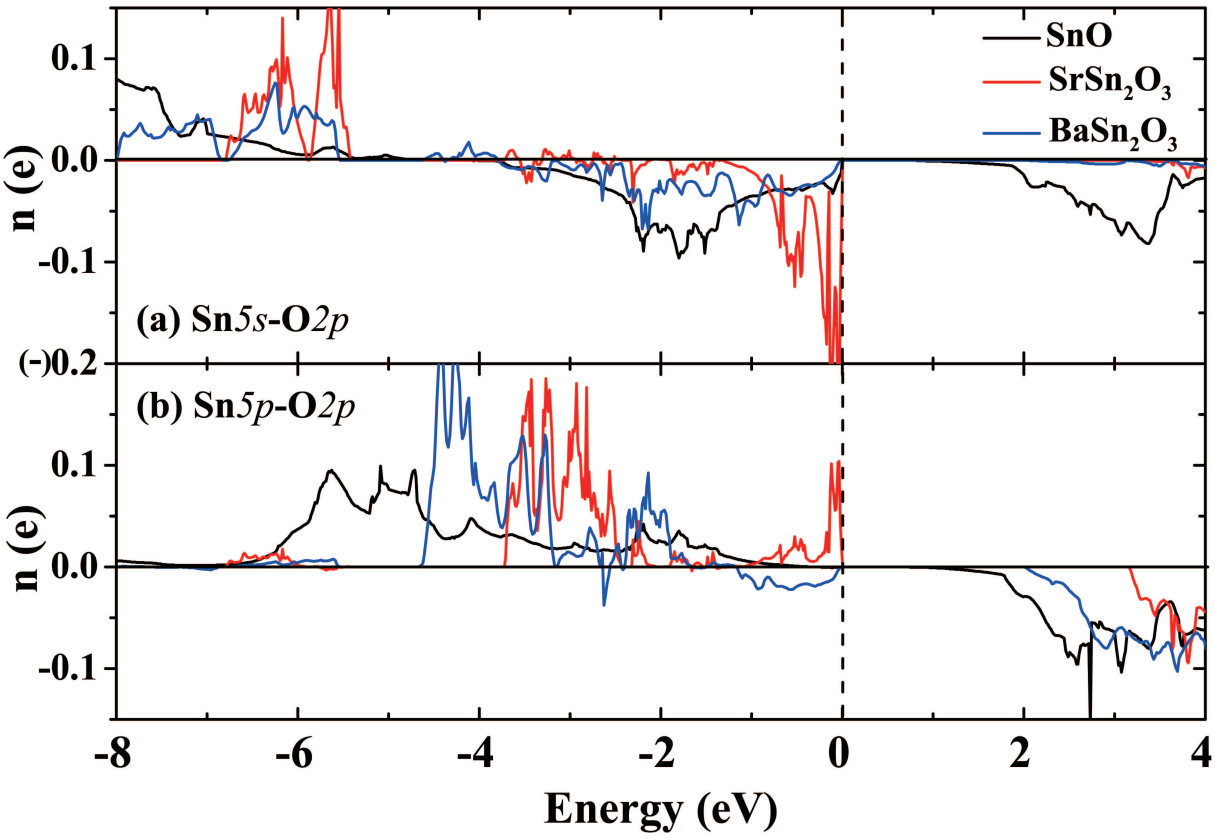

Figure S1: (Color online). Results of crystal orbital overlap population (COOP) between the (a) Sn-5*s* and O-2*p* and (b) Sn-5*p* and O-2*p* orbitals for SnO (black), $SrSn_2O_3$ (red) and $BaSn_2O_3$ (blue). The positive n(e) represents bonding states and the negative n(e) represent anti-bonding ones. The VB maximum is set to energy zero.

Table S1: Explicit structural data of the metastable phases of $BaSn_2O_3$ (shown in Fig. 8 of the main text) identified from structure searches. The differences in energy between these structures and the ground-state $C2/c$ structure are indicated (as "Relative energy").

Relative energy Space group	Lattice parameters (Å)	Wyckoff positions	Atoms	x	y	z
	$a = 6.3843$	4c	Ba	0.0000	0.9990	0.2500
47 meV/atom	$b = 9.8625$	8m	Sn	0.0000	0.3368	0.5035
Cmcm	$c = 8.2268$	8e	O1	0.7823	0.5000	0.5000
		4c	O2	0.0000	0.7138	0.2500
	a = 5.9318		Ba1	0.1855	0.1412	0.9022
	b = 6.0781		Sn1	0.1150	0.2482	0.3397
31 meV/atom	c = 8.3409	2i	Sn2	0.5599	0.3984	0.6883
P-1	$\alpha = 98.2931^\circ$		O1	0.8206	0.4305	0.1886
	$\beta = 88.3811^\circ$		O2	0.3550	0.3243	0.1906
	$\gamma = 60.8210^\circ$		O3	0.2478	0.8976	0.1684
			Ba	0.7725	0.6551	0.5937
	a = 10.5842		Sn1	0.8604	0.1622	0.8103
31 meV/atom	b = 5.9041	4c	Sn2	0.2110	0.1605	0.8373
*C*2	c= 14.6972		O1	0.1505	0.9507	0.6865
	$\beta = 145.4060^\circ$		O2	0.6025	0.9328	0.6907
			O3	0.8666	0.1143	0.6686
	a= 10.8670	4e	Ba	0.0000	0.7222	0.2500
25 meV/atom	b = 5.9815	8f	Sn	0.7222	0.0754	0.9962
$C2/c$	c = 13.8858	8f	O1	0.6256	0.8851	0.0183
	$\beta = 144.2090^\circ$	4e	O2	0.0000	0.5487	0.7500
			Ba1	0.0839	0.8568	0.1678
			Ba2	0.0165	0.9346	0.6692
			Sn1	0.3909	0.2241	0.3940
	a = 6.0895		Sn2	0.3517	0.2422	0.8750
	b = 6.1125		Sn3	0.7443	0.5338	0.9435
23 meV/atom	c = 8.1359	1a	Sn4	0.6908	0.5325	0.4619
*P*1	$\alpha = 91.7823^\circ$		O1	0.0519	0.1684	0.9493
	$\beta = 87.3882^\circ$		O2	0.7662	0.1577	0.4004
	$\gamma = 61.3076^\circ$		O3	0.3202	0.6018	0.4252
			O4	0.0440	0.6143	0.8960
			O5	0.6641	0.4707	0.7090
			O6	0.3357	0.1376	0.6311

Relative energy Space group	Lattice parameters (Å)	Wyckoff positions	Atoms	x	y	z
		2a	Ba1	0.0000	0.0040	0.0000
	a = 10.8670	2b	Ba2	0.5000	0.0037	0.5000
20 meV/atom	b = 5.9815	4c	Sn1	0.3930	0.0017	0.7196
$C2$	c = 13.8858	4c	Sn2	0.6187	0.4672	0.7998
	$\beta = 144.2090°$	4c	O1	0.5903	0.1281	0.7338
		4c	O2	0.3927	0.3466	0.7576
		4c	O3	0.8859	0.3721	0.0463
			Ba	0.4035	0.9072	0.8406
20 meV/atom	a = 9.7708		Sn1	0.6975	0.7327	0.5312
$Pca2_1$	b = 9.1720	4a	Sn2	0.8702	0.3714	0.3784
	c = 6.0581		O1	0.6994	0.8802	0.8095
			O2	0.2689	0.7295	0.1094
			O3	0.4970	0.1852	0.9377
		4d	Ba	0.2359	0.2500	0.7500
16 meV/atom	a = 11.2582	8e	Sn	0.9256	0.9931	0.7567
$Pnna$	b = 8.2117	4d	O1	0.3690	0.7500	0.2500
	c = 5.6619	8e	O2	0.8955	0.0231	0.1251
		2a	Ba1	0.0000	0.0000	0.0652
		2a	Ba2	0.0000	0.0000	0.5559
16 meV/atom	a = 10.9179	4c	Sn1	0.1749	0.4638	0.7823
$Pnn2$	b= 5.9425	4c	Sn2	0.6797	0.0072	0.8026
	c = 8.2892	4c	O1	0.8611	0.8611	0.8239
		4c	O2	0.1530	0.3988	0.5379
		4c	O3	0.1402	0.8458	0.3089
		4e	Ba	0.5000	0.2500	0.8077
11 meV/atom	a = 8.1110	8i	Sn	0.2549	0.2500	0.3998
$Imma$	b = 6.2523	4e	O1	0.5000	0.2500	0.0640
	c = 10.6876	8g	O2	0.2500	0.5255	0.7500
	a = 6.0678		Ba	0.4619	0.4594	0.7543
	b = 6.1860		Sn1	0.1571	0.8544	0.0364
9 meV/atom	c = 8.2778	2i	Sn2	0.8547	0.2166	0.4317
P-1	$\alpha = 97.1624°$		O1	0.7782	0.5118	0.5240
	$\beta = 90.7640°$		O2	0.7805	0.7862	0.9974
	$\gamma = 115.5592°$		O3	0.7866	0.2698	0.1962