

## SUPPORTING INFORMATION

# Structural Differences Between Sb- and Nb-Doped Tin Oxides and Consequences for Electrical Conductivity

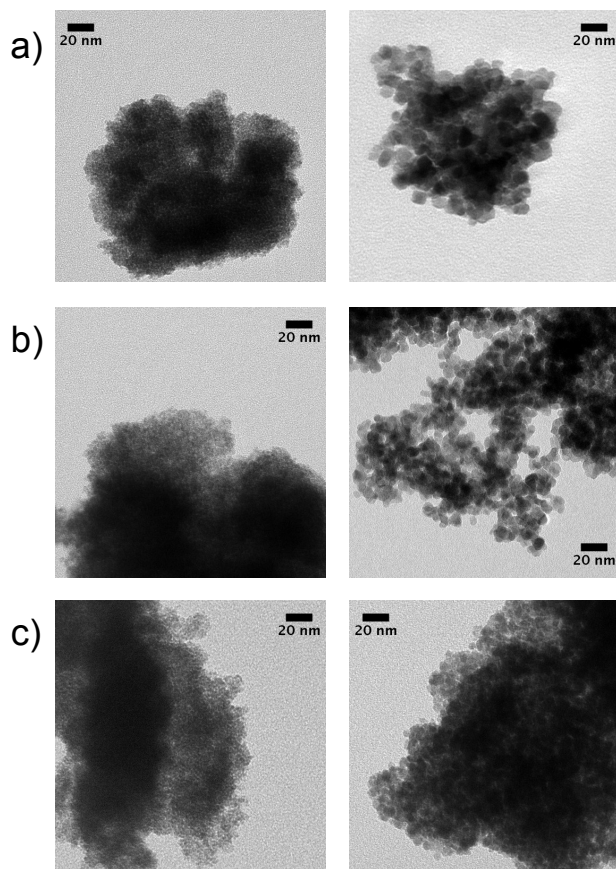
E. Oakton,<sup>a</sup> J. Tillier,<sup>b</sup> G. Siddiqi,<sup>a</sup> Z. Mickovic,<sup>b</sup> O. Sereda,<sup>b</sup> A. Fedorov,<sup>a</sup> and C. Copéret<sup>a\*</sup>

<sup>a</sup> ETH Zürich, Department of Chemistry and Applied Biosciences, Vladimir Prelog Weg 2, CH-8093 Zürich, Switzerland. Fax: 41 44 633 1325; Tel: 41 44 633 9394; E-mail: ccoperet@inorg.chem.ethz.ch

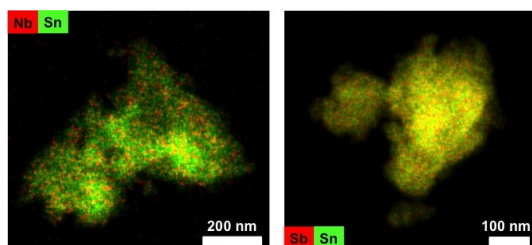
<sup>b</sup> CSEM SA, XRD Application Lab & Microscopy, Jaquet-Droz 1, CH-2002, Neuchâtel, Switzerland.

### Characterisation data

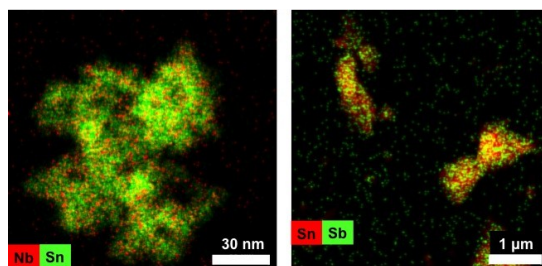
<b>Figure S1.</b> Representative Bright Field TEM images of a) SnO <sub>2</sub> , b) SnO <sub>2</sub> :Sb and c) SnO <sub>2</sub> :Nb before (left) and after (right) calcination	2
<b>Figure S2.</b> EDX maps of SnO <sub>2</sub> :Nb (left) and SnO <sub>2</sub> :Sb (right) before calcination	2
<b>Figure S3.</b> EDX maps of SnO <sub>2</sub> :Nb (left) and SnO <sub>2</sub> :Sb (right) after calcination	2
<b>Figure S4.</b> Representative N <sub>2</sub> adsorption desorption isotherms of SnO <sub>2</sub> :Sb	3
<b>Figure S5.</b> XRD powder diffraction patterns of SnO <sub>2</sub> (green), SnO <sub>2</sub> :Sb (blue) and SnO <sub>2</sub> :Nb (black) measured on a glass substrate at room temperature after the HT-XRD measurements	3
<b>Figure S6.</b> XRD powder diffraction patterns of SnO <sub>2</sub> , SnO <sub>2</sub> :Sb and SnO <sub>2</sub> :Nb before calcination (black) and at 500 °C (blue)	4
<b>Figure S7.</b> HT-XRD diffraction patterns of SnO <sub>2</sub> during heating cycle 1	5
<b>Figure S8.</b> HT-XRD diffraction patterns of SnO <sub>2</sub> during heating cycle 2	5
<b>Figure S9.</b> HT-XRD diffraction patterns of SnO <sub>2</sub> :Sb during heating cycle 1	6
<b>Figure S10.</b> HT-XRD diffraction patterns of SnO <sub>2</sub> :Sb during heating cycle 2	6
<b>Figure S11.</b> HT-XRD diffraction patterns of SnO <sub>2</sub> :Nb during heating cycle 1	7
<b>Figure S12.</b> HT-XRD diffraction patterns of SnO <sub>2</sub> :Nb during heating cycle 2	7
<b>Table S1.</b> Elemental analysis data for SnO <sub>2</sub> :Sb and SnO <sub>2</sub> :Nb (wt%)	8
<b>Table S2.</b> Surface area and electrical conductivity data of the SnO <sub>2</sub> :Sb samples	8
<b>Table S3.</b> Surface area and electrical conductivity data of the SnO <sub>2</sub> :Nb samples with varied Nb content calcined at 500 °C	8
<b>Table S4.</b> Surface area and electrical conductivity data of the 5 mol <sub>M</sub> % SnO <sub>2</sub> :Nb samples with varied calcination temperatures	9



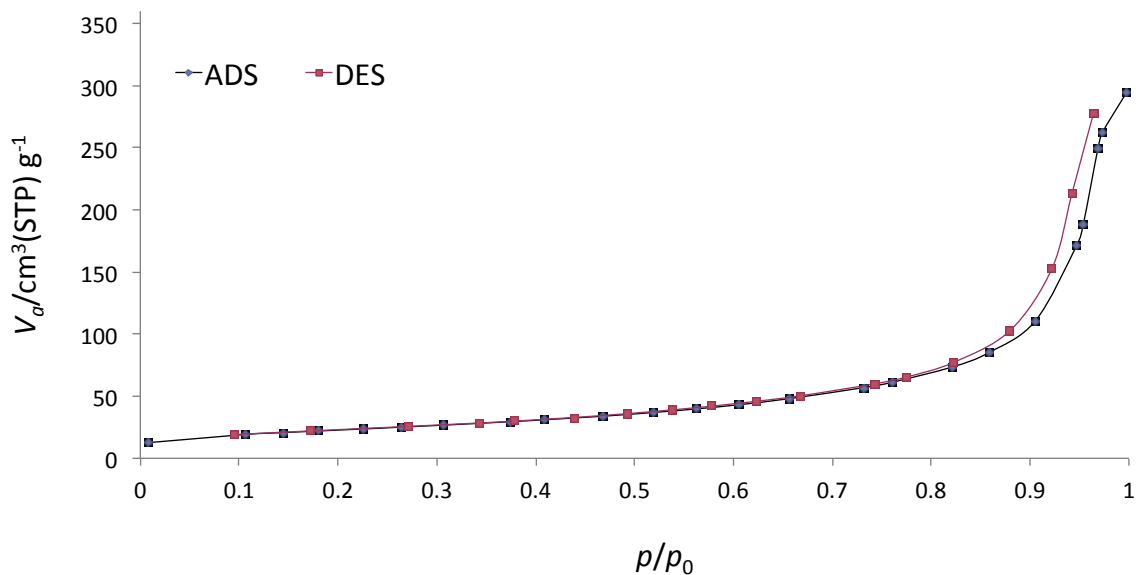
**Figure S1.** Representative Bright Field TEM images of a)  $\text{SnO}_2$ , b)  $\text{SnO}_2:\text{Sb}$  and c)  $\text{SnO}_2:\text{Nb}$  before (left) and after (right) calcination



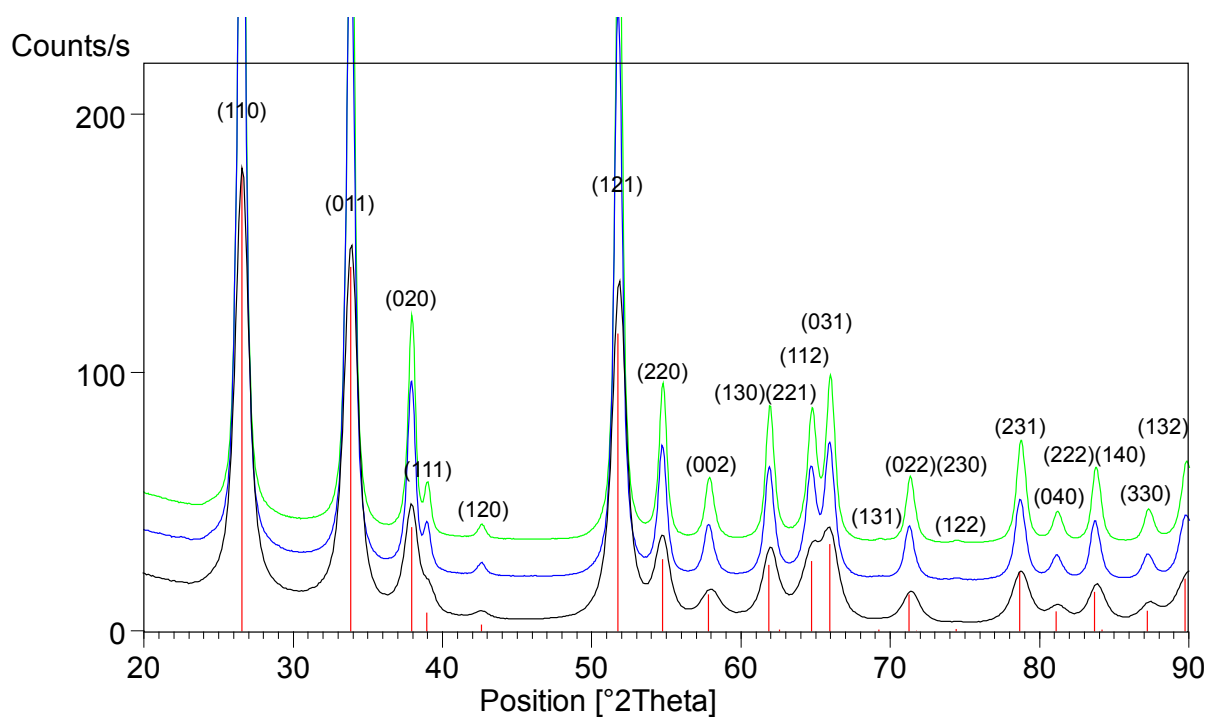
**Figure S2.** EDX maps of  $\text{SnO}_2:\text{Nb}$  (left) and  $\text{SnO}_2:\text{Sb}$  (right) before calcination



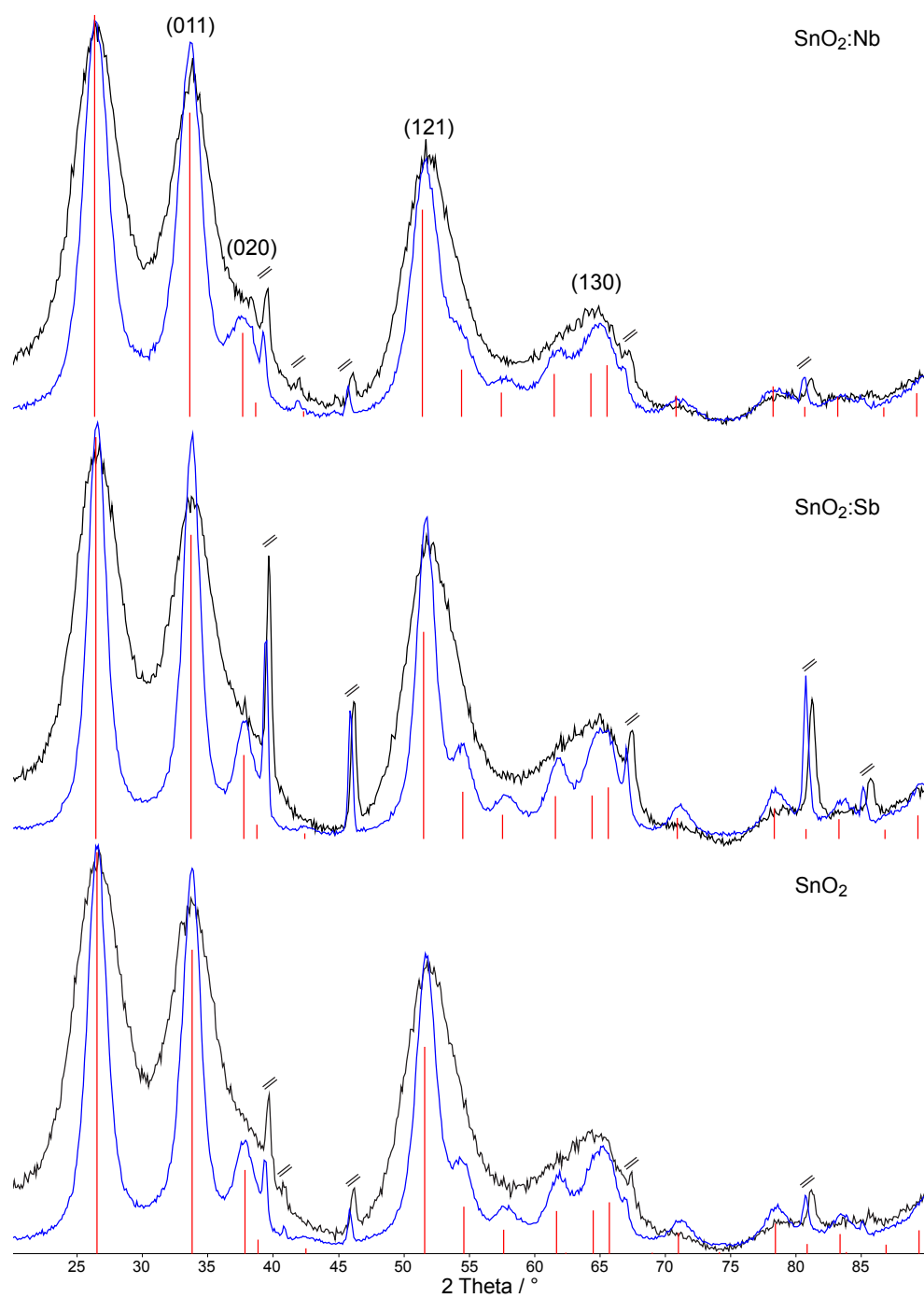
**Figure S3.** EDX maps of  $\text{SnO}_2:\text{Nb}$  (left) and  $\text{SnO}_2:\text{Sb}$  (right) after calcination



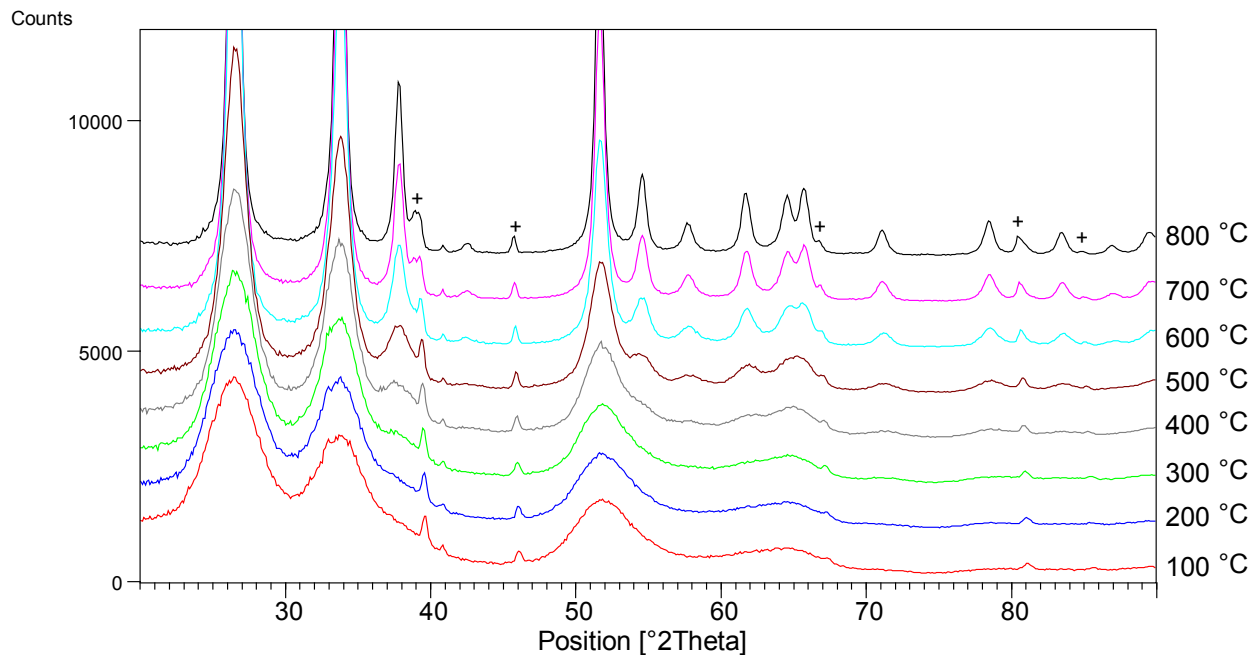
**Figure S4.** Representative  $N_2$  adsorption-desorption isotherms of  $SnO_2:Sb$



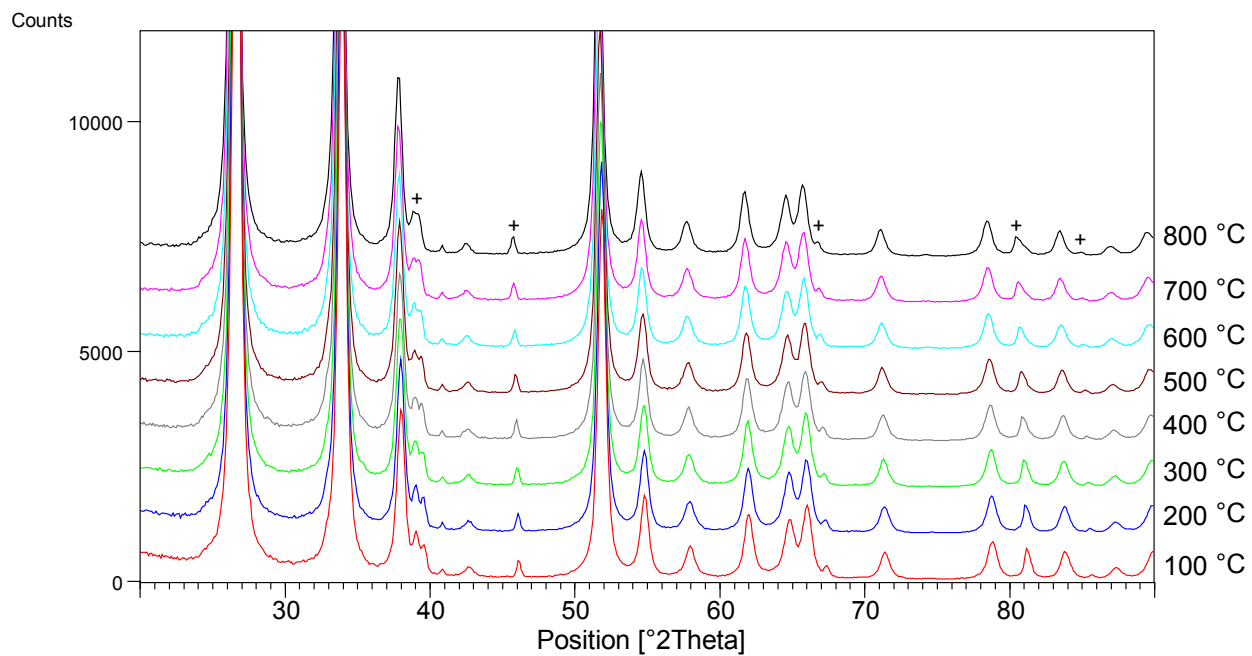
**Figure S5.** XRD powder diffraction patterns of  $SnO_2$  (green),  $SnO_2:Sb$  (blue) and  $SnO_2:Nb$  (black) measured on a glass substrate at room temperature after the HT-XRD measurements. The red lines represent the theoretical peak positions of Cassiterite  $SnO_2$ . Major diffraction peaks are indexed ( $hkl$ ) and assigned to cassiterite  $SnO_2$ .



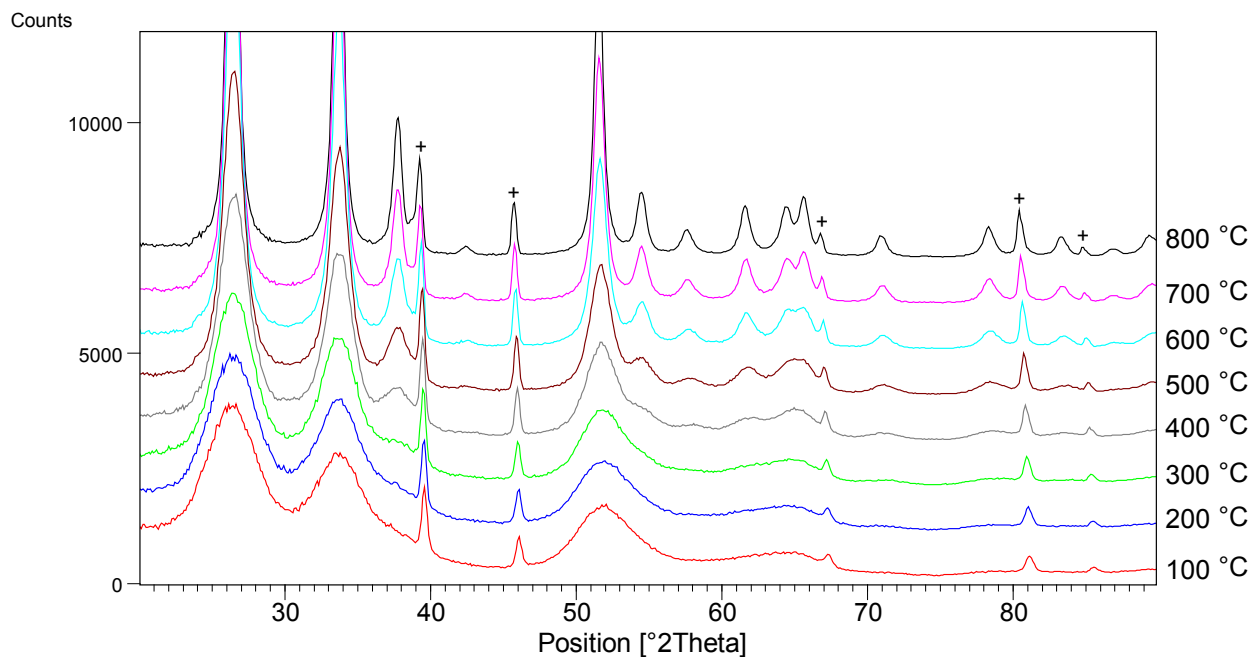
**Figure S6.** XRD powder diffraction patterns of  $\text{SnO}_2$ ,  $\text{SnO}_2\text{:Sb}$  and  $\text{SnO}_2\text{:Nb}$  before calcination (black) and at  $500\text{ }^\circ\text{C}$  (blue). Red lines represent the theoretical peak positions of cassiterite  $\text{SnO}_2$ . Double line represent peaks due to the Pt heating strip. A small shift in the peaks assigned to the Pt heating strip is observed due to thermal expansion for the diffractograms recorded at  $500\text{ }^\circ\text{C}$  (blue). Major diffraction peaks are indexed ( $hkl$ ).



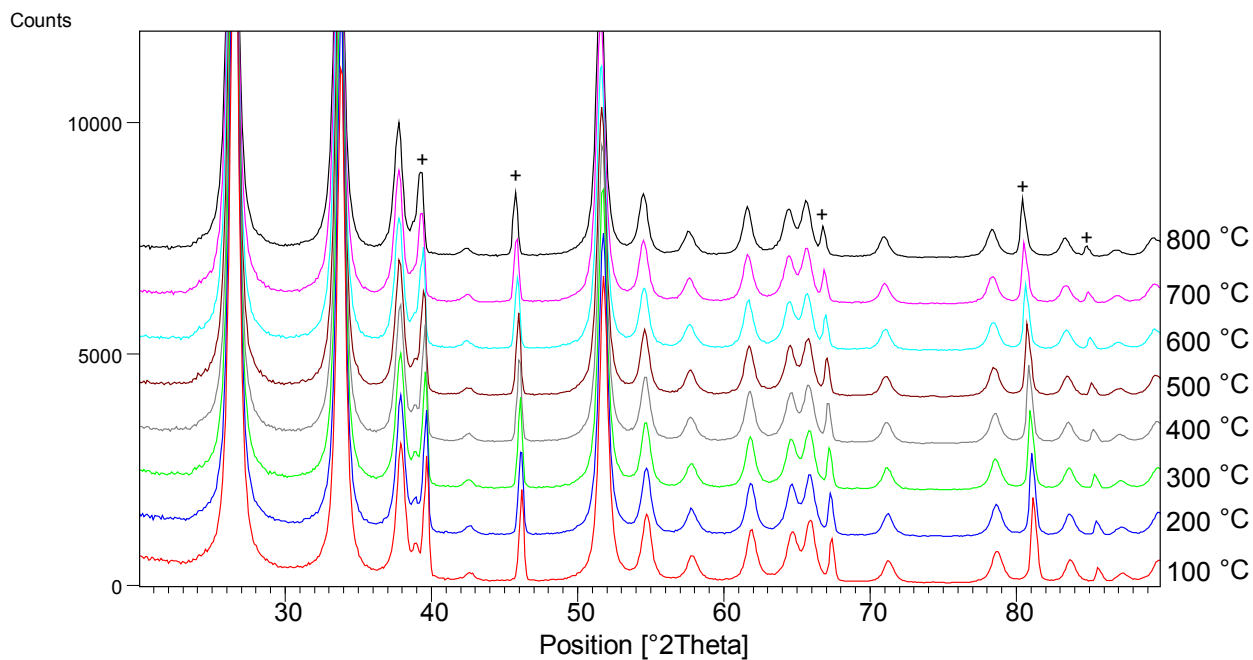
**Figure S7.** HT-XRD diffraction patterns of SnO<sub>2</sub> during heating cycle 1. Peaks due to the Pt heating strip are denoted by a + sign. All others correspond to cassiterite SnO<sub>2</sub>.



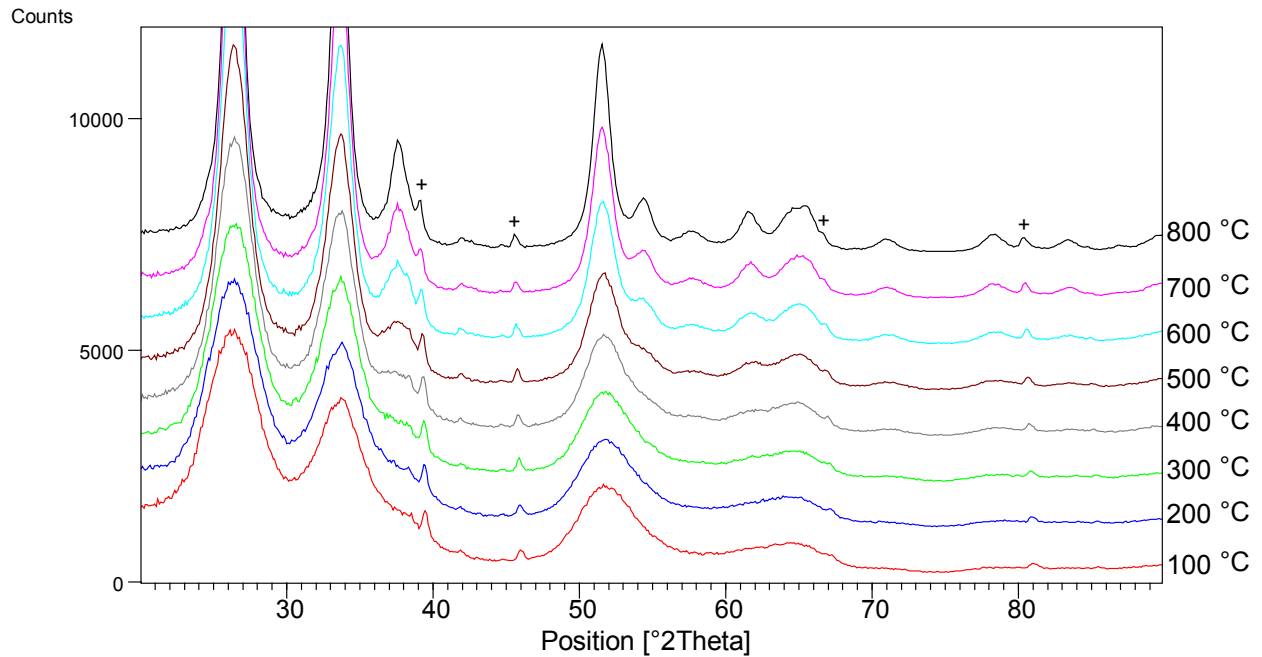
**Figure S8.** HT-XRD diffraction patterns of SnO<sub>2</sub> during heating cycle 2. Peaks due to the Pt heating strip are denoted by a + sign. All other corresponds to cassiterite SnO<sub>2</sub>.



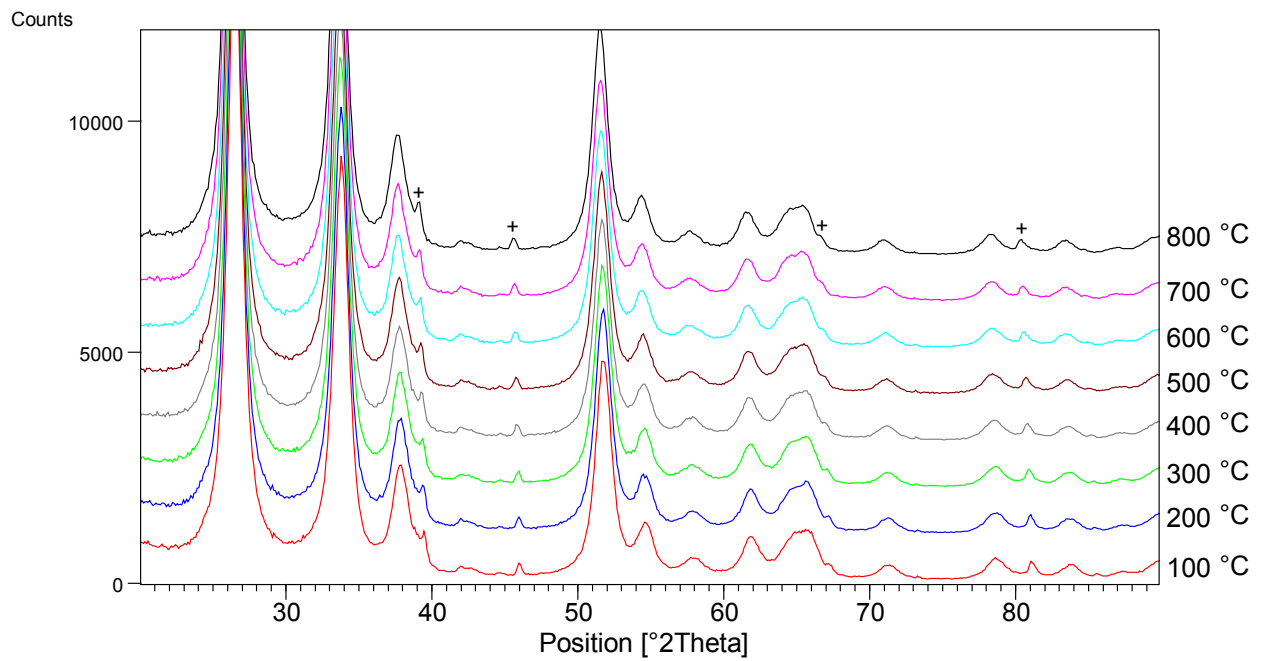
**Figure S9.** HT-XRD diffraction patterns of SnO<sub>2</sub>:Sb during heating cycle 1. Peaks due to the Pt heating strip are denoted by a + sign. All others correspond to cassiterite SnO<sub>2</sub>.



**Figure S10.** HT-XRD diffraction patterns of SnO<sub>2</sub>:Sb during heating cycle 2. Peaks due to the Pt heating strip are denoted by a + sign. All others correspond to cassiterite SnO<sub>2</sub>.



**Figure S11.** HT-XRD diffraction patterns of  $\text{SnO}_2\text{:Nb}$  during heating cycle 1. Peaks due to the Pt heating strip are denoted by a + sign. All others correspond to cassiterite  $\text{SnO}_2$ .



**Figure S12.** HT-XRD diffraction patterns of  $\text{SnO}_2\text{:Nb}$  during heating cycle 2. Peaks due to the Pt heating strip are denoted by a + sign. All others correspond to cassiterite  $\text{SnO}_2$ .

**Table S1.** Elemental analysis data for SnO<sub>2</sub>:Sb and SnO<sub>2</sub>:Nb (wt%)

Sample	Sn	Sb	Nb	Cl
SnO <sub>2</sub> :Sb	73.2	1.92	-	0.53
SnO <sub>2</sub> :Nb	70.5	-	2.97	1.18

**Table S2.** Surface area and electrical conductivity data of the SnO<sub>2</sub>:Sb samples

Sample	Calcination / T °C	S <sub>BET</sub> / m <sup>2</sup> .g <sup>-1</sup>	Electrical conductivity / S.cm <sup>-1</sup>
SnO <sub>2</sub> :Sb	500	83	0.02
Commercial SnO <sub>2</sub> :Sb	-	70-80	0.03

**Table S3.** Surface area and electrical conductivity data of the SnO<sub>2</sub>:Nb samples with varied Nb content calcined at 500 °C

Nb content / mol <sub>M</sub> %	S <sub>BET</sub> / m <sup>2</sup> .g <sup>-1</sup>	Electrical conductivity / S.cm <sup>-1</sup>
0	33	10 <sup>-6</sup>
1	28	10 <sup>-6</sup>
2	28	10 <sup>-6</sup>
5	43	10 <sup>-5</sup>
10	55	10 <sup>-6</sup>



**Table S4.** Surface area and electrical conductivity data of the 5 mol<sub>M</sub>% SnO<sub>2</sub>:Nb samples with varied calcination temperatures

Calcination T / °C	S <sub>BET</sub> / m <sup>2</sup> .g <sup>-1</sup>	Electrical conductivity / S.cm <sup>-1</sup>
-	257	10 <sup>-7</sup>
350	143	10 <sup>-6</sup>
500	92	10 <sup>-5</sup>
650	59	10 <sup>-5</sup>
800	28	10 <sup>-6</sup>