Supporting Information

Electron/hole pinning effect, localization, and dielectric properties in (Nb, Cu) co-doped SnO_2 ceramics

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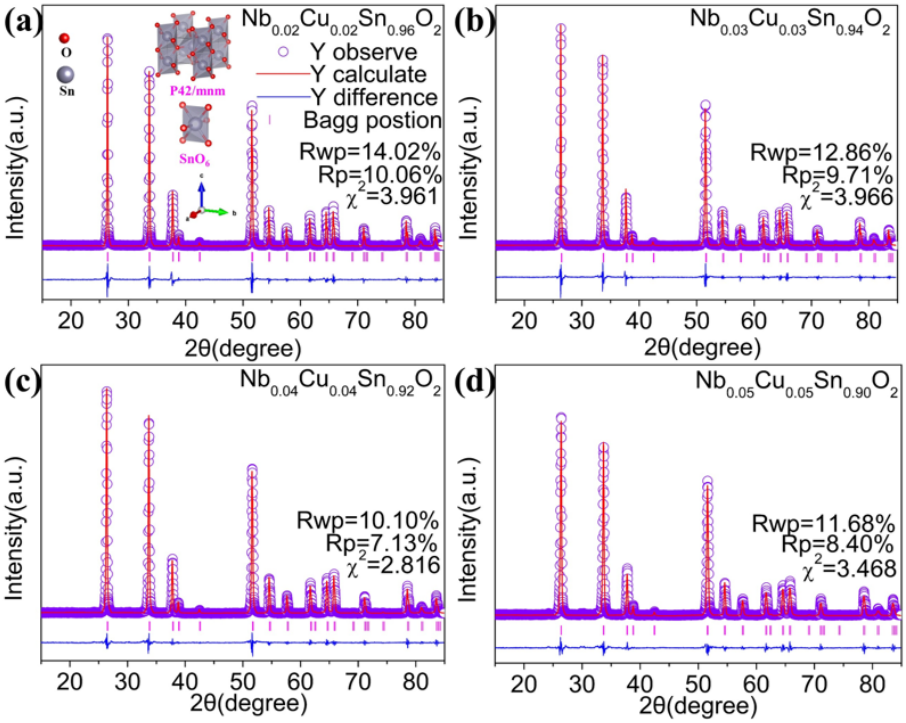

Figure S1 XRD refinement patterns of (Nb, Cu) co-doped SnO_2 samples. (a) N2C2SO, (b) N3C3SO; (c) N4C4SO; (d) N5C5SO, inset in (a) showed the lattice structure of SnO_2.

Table S1 The lattice parameters and volumes of the $Nb_xCu_ySn_{1-x-y}O_2$ samples from the XRD refinement.

Composition	a(Å)	b(Å)	c(Å)	Volume(Å)	Bond length(Å)	R_p	R_{wp}	χ^2
SO	4.7388	4.7388	3.1868	71.563	2.0519	7.54%	11.16%	3.977
N2SO	4.7381	4.7381	3.1862	71.529	2.0515	6.68%	8.83%	3.474
C2SO	4.7413	4.7413	3.1890	71.688	2.0531	11.12%	15.54%	4.128
N1C1SO	4.7409	4.7409	3.1882	71.656	2.0527	10.04%	16.13%	3.601
N2C2SO	4.7422	4.7422	3.1886	71.708	2.0532	10.06%	14.02%	3.961
N3C3SO	4.7434	4.7434	3.18953	71.764	2.0537	9.71%	12.86%	3.966
N4C4SO	4.7420	4.7420	3.1881	71.689	2.0529	7.13%	10.10%	2.816
N5C5SO	4.7415	4.7415	3.1876	71.661	2.0526	8.40%	11.68%	3.468

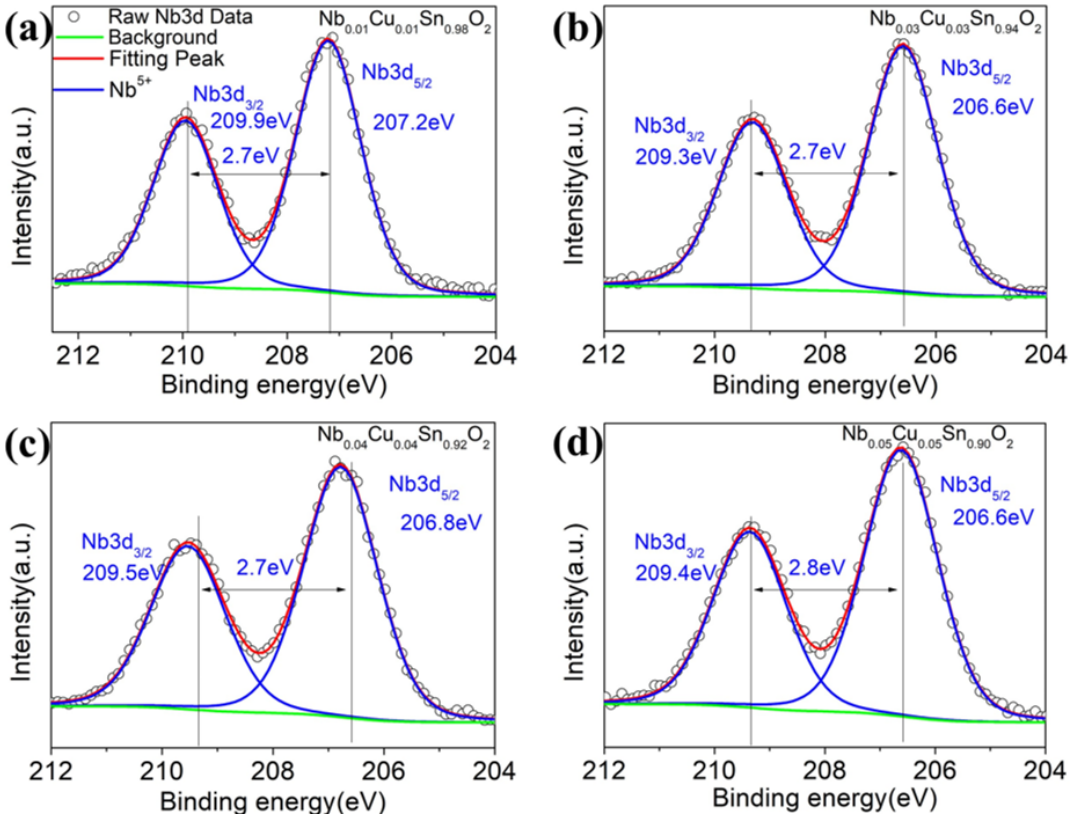

Figure S2 XPS of Nb 3d in all compositions of (a)N1C1SO; (b)N3C3SO; (c)N4Z4SO; (d)N5Z5SO.

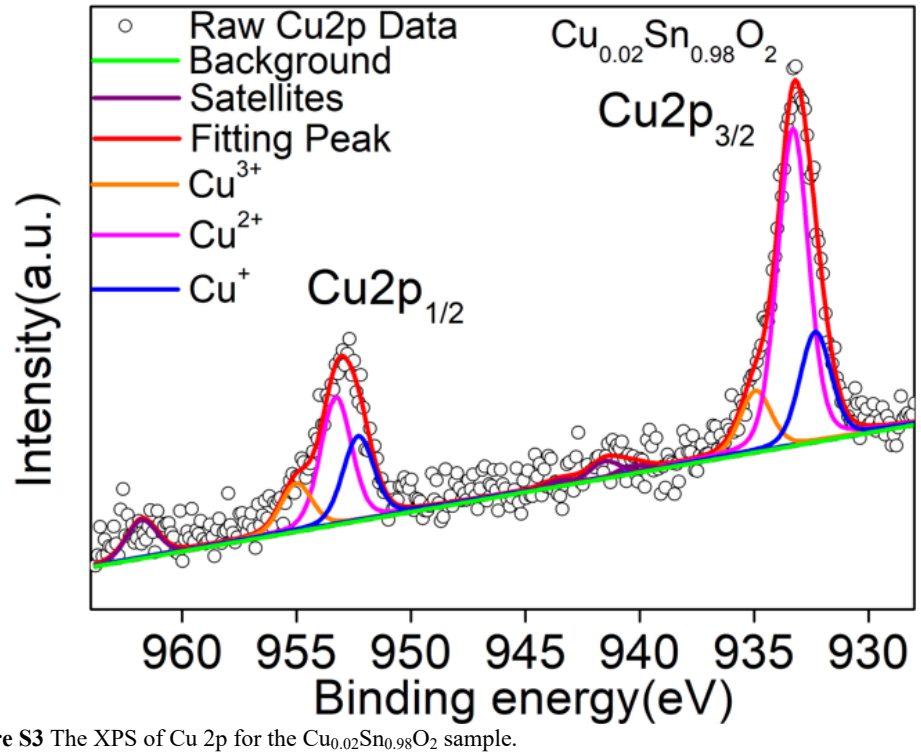

Figure S3 The XPS of Cu 2p for the $Cu_{0.02}Sn_{0.98}O_2$ sample.

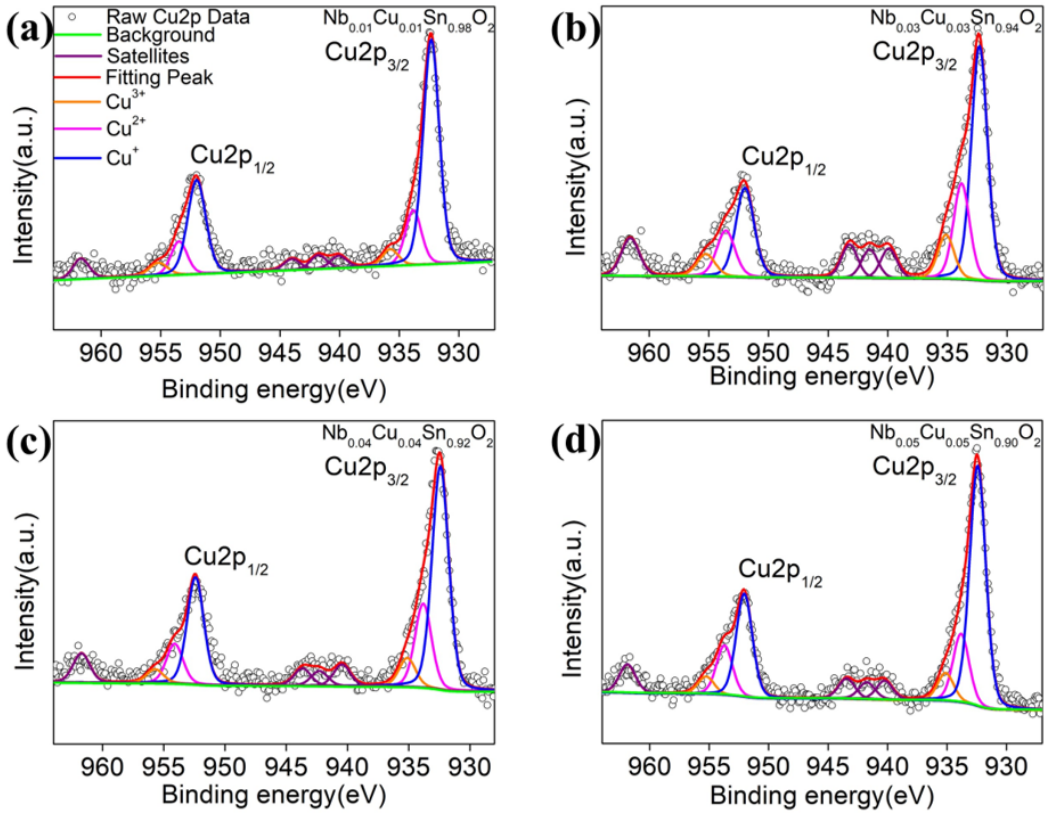

Figure S4 The XPS of Cu 2p for the NCSO samples, (a) N1C1SO, (b) N3C3SO, (c) N4C4SO, and (d) N5C5SO.

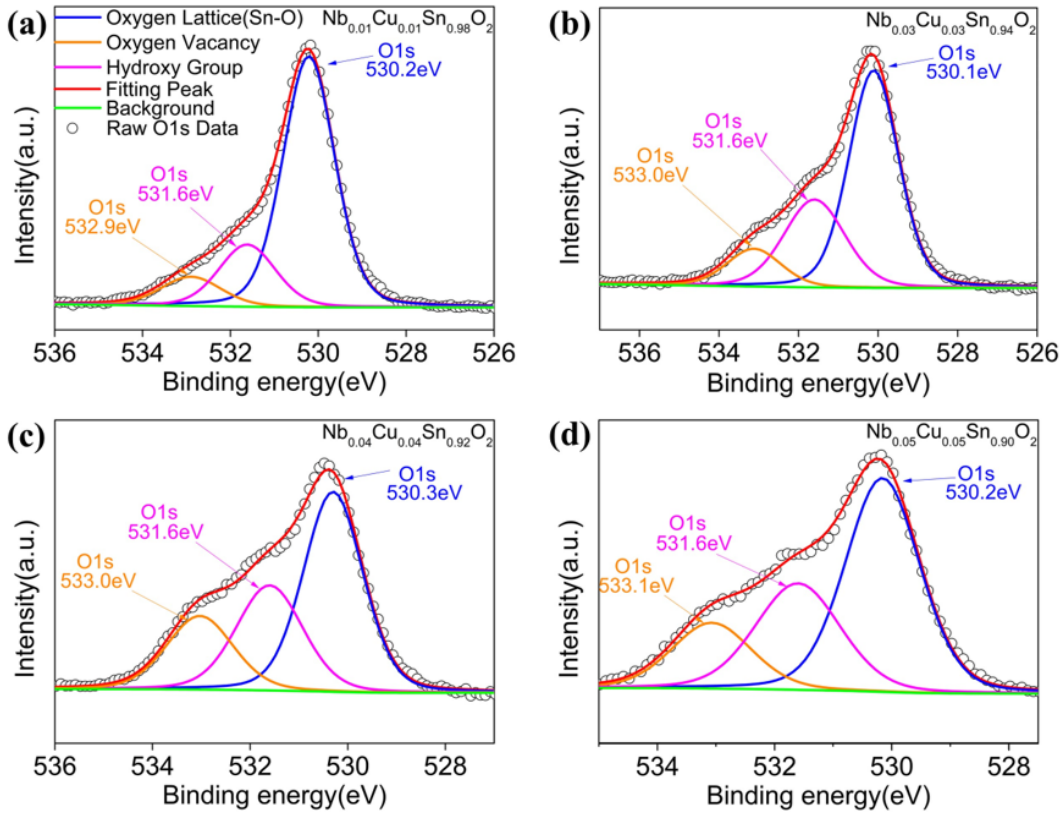

Figure S5 XPS of O 1s in co-doped NCSO. (a) N1C1SO; (b) N3Z3SO; (c) N3C3SO; (d) N5C5SO.

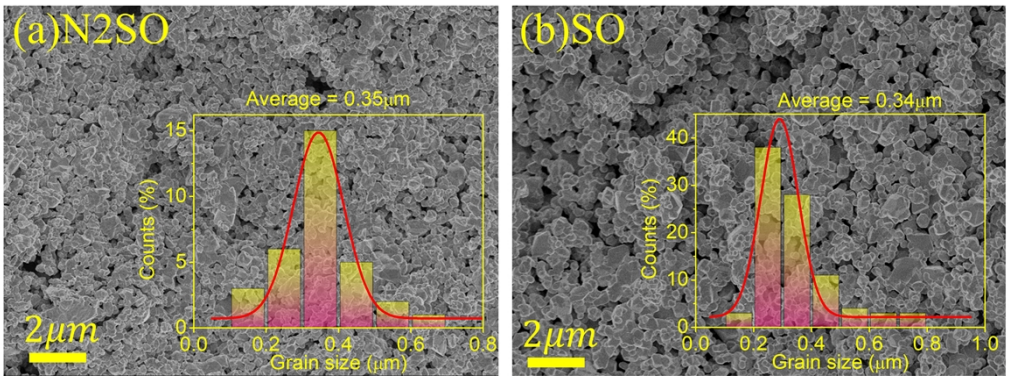

Figure S6 SEM morphologies of (a) N2SO and (b) SO from previous work (ref [1]), insets give the size distribution.

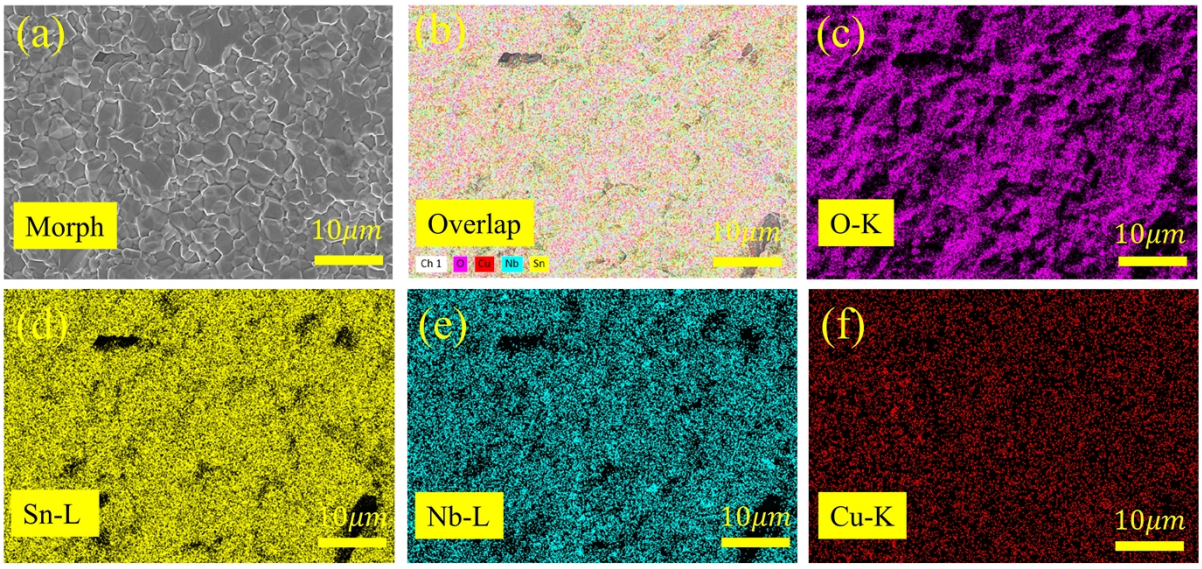

Figure S7 Elemental mapping images of the N1C1SO ceramic.

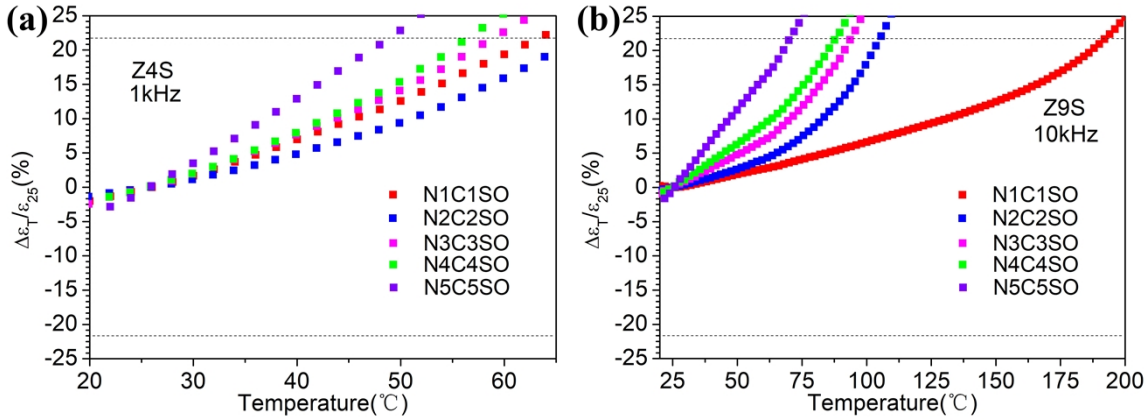

Figure S8 Temperature coefficients of dielectric constant for NCSO ceramics, (a) 1 kHz, and (b) 10 kHz.

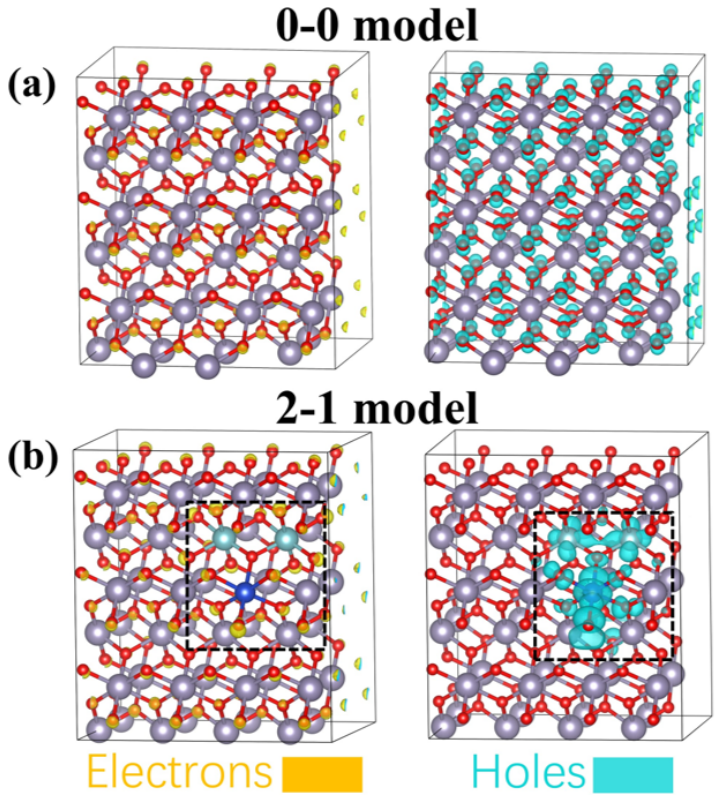

Figure S9 The iso-surface of electrons and holes of excitation state in (Nb, Cu) co-doped SnO_2 (3 × 2 × 4 supercell). (a) pure SnO_2, and (b) co-doped SnO_2, two Nb adjacent to one Cu (2-1 model).

Table S2 The Hole Delocalization Index (HDI) and Electron Delocalization Index (EDI) of partial atomic excitation state from pure SnO_2 (0-0 model).

Element-Number	HDI	EDI
Sn-35	0.00	0.11
O-83	0.36	0.13
O-92	0.36	0.13
O-102	0.36	0.13
O-107	0.36	0.13
O-116	0.36	0.13
O-117	0.36	0.13

Table S3 The HDI and EDI of partial atomic excitation state from Nb doped SnO_2 (1-0 model).

Element-Number	HDI	EDI
O-78	0.12	0.22
O-87	0.12	0.22
O-97	0.12	0.22
O-102	0.12	0.22
O-111	0.12	0.22
O-112	0.12	0.22
O-92 (Not near Nb)	0.47	0.13
O-116 (Not near Nb)	0.43	0.14
Nb-144	0.00	0.07

Table S4 The HDI and EDI of partial atomic excitation state from Cu doped SnO_2 (0-1 model).

Element-Number	HDI	EDI
Sn-46	0.00	0.17
O-82	**3.41**	1.30
O-91	**3.31**	0.18
O-101	1.31	0.29
O-106	0.59	0.22
O-115	1.62	0.29
Cu-143	0.04	3.61

Table S5 The HDI and EDI of partial atomic excitation state from (Nb+Cu) co-doped SnO_2 (1-1 model).

Element-Number	HDI	EDI
Sn-34	0.61	0.07
O-81	0.23	0.42
O-90	0.32	1.06
O-100	0.20	0.52
O-105	0.32	0.64
O-111	0.47	0.09
O-112	0.45	0.09
O114	0.17	0.50
O-128	0.15	0.72
O-134	0.57	0.22
O-135	0.55	0.22
Cu-142	1.64	**15.82**
Nb-143	0.80	**5.69**

Table S6 The HDI and EDI of partial atomic excitation state from (Nb+Cu) co-doped SnO_2 (2-2 model).

Element-Number	HDI	EDI
O-79	0.01	0.27
O-85	0.56	0.17
O-86	0.14	0.16
O-87	0.18	0.22
O-88	0.03	0.21
O-98	0.01	0.23
O-103	0.03	0.10
O-109	**2.57**	0.10
O-110	**3.17**	0.17
O-111	0.10	0.06
O-112	0.01	0.28
O-115	0.00	0.14
O-121	0.01	0.24
O-126	0.01	0.26
O-132	**6.22**	0.33
O-133	0.17	0.17
O-135	0.11	0.20
O-136	0.01	0.28
Cu-140	**1.46**	0.09
Cu-141	**24.03**	0.92
Nb-142	0.12	0.06
Nb-143	0.03	0.08

Table S7 The HDI and EDI of partial atomic excitation state from (Nb+Cu) co-doped SnO_2 (2-1 model).

Element-Number	HDI	EDI
O-80	0.01	0.26
O-89	0.16	0.21
O-99	0.01	0.20
O-104	0.23	0.14
O-110	0.50	0.15
O-111	0.96	0.15
O-112	**4.49**	0.36
O113	0.40	0.03
O-114	0.00	0.25
O-123	0.01	0.20
O-128	0.01	0.26
O-130	0.01	0.13
O-134	1.02	0.15
O-135	0.45	0.15
O-137	0.16	0.21
O-138	0.00	0.25
Cu-142	**31.51**	0.20
Nb-143	0.90	0.06
Nb-144	0.90	0.06

References

1 Y. Tan, H. Wang, Y. Wang, Y. Ren, J. Wen, J. Ma, Y. Ma, D. Xu, Y. Yue and B. Wang, *Ceram. Int.*, 2023, **49**, 21402-21410.