Supporting Information

Application of Transient IR Spectroscopy to Investigate the Role of Gold in Ethanol Gas Sensing over Au/SnO_2

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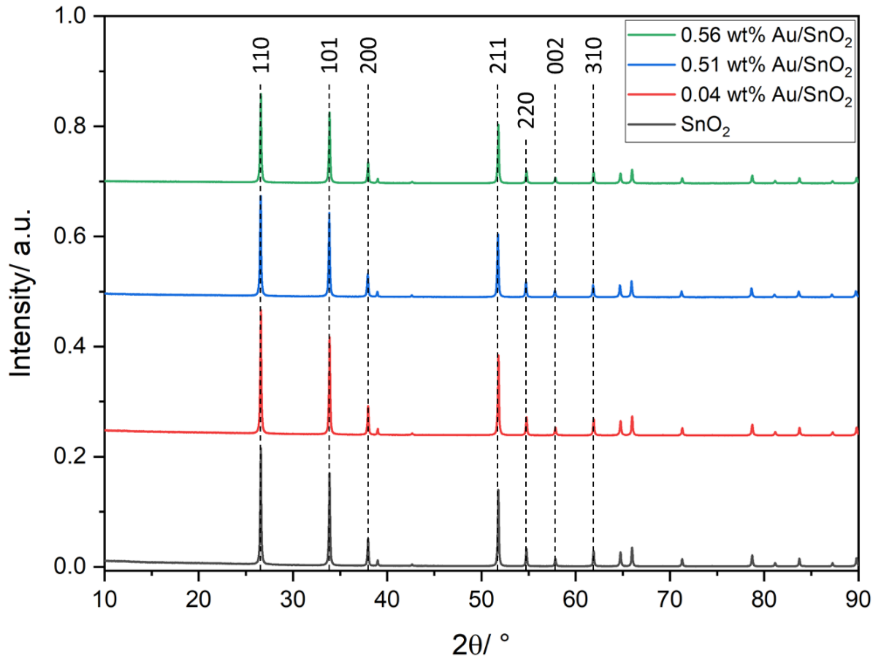

Figure S1. X-ray powder diffractograms of the samples using Cu K_α-radiation (1.5406 Å, 40 kV, 40 mA).

Table S1. Composition of bare and gold-loaded tin oxide materials used in this work.

Sample name	XPS						ICP-OES
	x(C)/ at%	x(O)/ at%	x(Sn)/ at%	x(Au)/ at%	w(Au)/ wt%	O/Sn	w(Au)/ wt%
SnO_2	5.2	59.7	35.1	0.0	0.00	1.70	0.00
0.04 wt% Au/SnO_2	13.0	56.3	30.7	0.0	0.00	1.83	0.04
0.51 wt% Au/SnO_2	7.2	58.6	33.7	0.5	1.92	1.74	0.51
0.56 wt% Au/SnO_2	9.1	57.2	33.2	0.6	2.17	1.72	0.56

Table S2. Mean crystallite sizes and specific surface areas of bare and gold-loaded tin oxide samples, as determined from X-ray diffraction and N_2 physisorption measurements.

Probe	**Mean crystallite size d/ nm**	**Specific surface area/ $m^2 \cdot g^{-1}$**
SnO_2	59.0	25.0
0.04 wt% Au/SnO_2	57.0	17.3
0.51 wt% Au/SnO_2	59.1	19.8
0.56 wt% Au/SnO_2	57.0	25.5

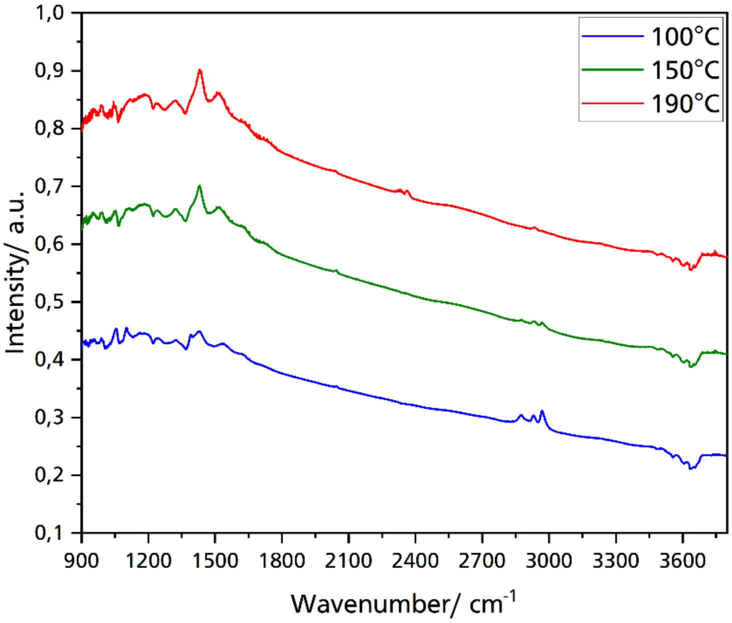

Figure S2. Exemplary DRIFT spectrum of 0.56 wt% Au/SnO_2 during exposure to 500 ppm ethanol at operating temperatures of 100°C, 150°C, and 190°C.

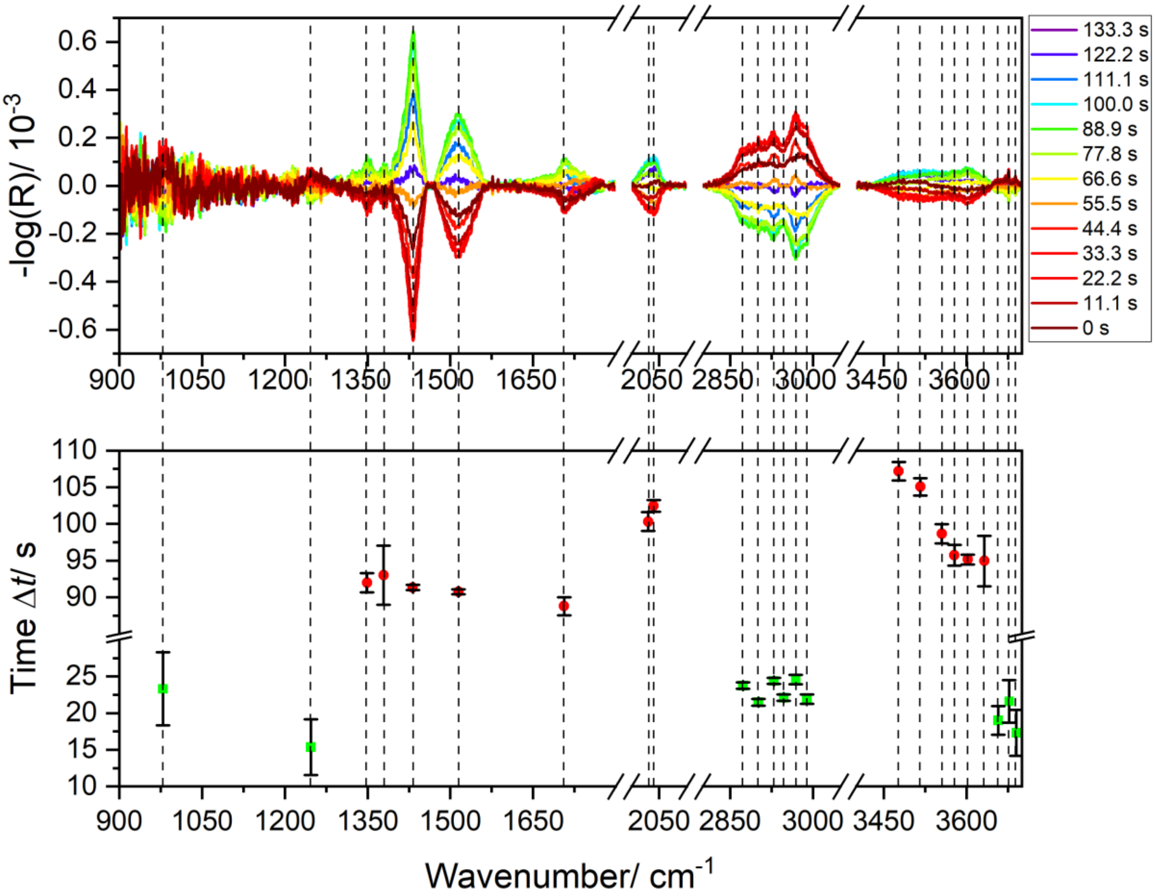

Figure S3. Temporal analysis of PSD spectra for 0.56 wt% Au/SnO_2 during pulsing of 500 ppm ethanol in synthetic air at 150°C. Time values Δt (bottom panel) were calculated from the phase angles at maximum band intensity. Dashed lines indicate the maxima of observed features and their corresponding time values. Time values in the first half-period are colored green, those in the second half-period are colored red. The error bars show the standard deviation of the time values Δt within the range of ±5 cm^{-1} with respect to the position of the maximum.

Table S3. Band assignment based on results of time-resolved DRIFTS measurements and observations in the literature; T: terminal; B: bridged.

Band position/ cm^{-1}	Band assignment	Literature
934	δ(Sn-OH)(T)	1–3
979	δ(Sn-OH)(T)	1,4,5
1100	ν(C-O) ethoxy	6,7
1247	δ(Sn-OH)(T)	2,4,5
1349	ν_s(COO) carboxylate	4,8,9
1379	ν_s(COO) carbonate	3,4,8,9
1432	ν_{as}(COO) carbonate	3,4,8,9
1515	ν_{as}(COO) carboxylate	4,8,9
1626	δ(HOH) H_20_{ads}	1,8,10,11
1706	*ν*(C=O) acetaldehyde)	12,13
2040	CO-$Au^{\delta-}$	14–16
2349	ν_{as}(OCO) $CO_{2, gas}$	3,17–19
2873	$\nu_s(CH_3)$ acetate, ethoxy *ν*(C-H) formate	12,14,20–22
2901	$\nu_{as}(CH_2)$ adsorbed ethanol	12,14,20–22
2929	$\nu_{as}(CH_2)$ ethoxy	12,14,20–22
2947	$\nu_{as}(CH_2)$ ethanol	12,14,20–22
2969	$\nu_{as}(CH_3)$ acetate, ethoxy *ν*(C-H) formate	12,14,20–22
2989	$\nu_{as}(CH_3)$ ethanol	12,14,20–22
3460	*ν*(OH)(B)	1,10,23–25
3555	*ν*(OH)(B)	1,10,23–25
3604	*ν*(OH)(T)	1,10,23–25
3631	*ν*(OH)(T)	1,10,23–25
3636	*ν*(OH)(T)	1,10,23–25
3652	*ν*(OH)(T)	1,10,23–25
3673	*ν*(OH)(T)	1,10,23–25

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