

Supplementary Information

Precisely Tailored LaFeO₃ Dendrites using Urea and Piperazine Hexahydrate for Highly Sensitive, Selective and Trace Level Detection of Acetone

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Table S1. Detailed reactant concentrations and corresponding outcomes

S. No	Sample code	Piperazine hexahydrate mM [mg]	Urea mM [mg]	Before/ After pH	Crystalline Phase	Morphology
1	U9	0	9 (540.54)	2.67/9.30	LaFeO ₃	Irregular Particle with Aggregation
2	U9P3	3 (582.69)	9 (540.54)	6.74/9.35	La(OH) ₃ , LaFeO ₃	Parallelogram and Irregular Structures
3	U9P6	6 (1165.38)	9 (540.54)	9.49/9.56	LaFeO ₃	Dendritic Growth Initiation
4	U9P9	9 (1748.07)	9 (540.54)	9.54/9.60	LaFeO ₃	Early - Stage Dendrites
5	U9P12	12 (2330.76)	9 (540.54)	9.88/9.92	LaFeO ₃	Mid - Stage Dendrites
6*	U9P15	15 (2913.45)	9 (540.54)	9.90/9.90	LaFeO ₃	Fully Grown Dendrites
7	U9P18	18 (3496.14)	9 (540.54)	10.01/10.03	LaFeO ₃	Fully Grown Dendrites
8	U9P21	21 (4078.83)	9 (540.54)	10.10/10.12	LaFeO ₃	Fully Grown Dendrites
9	P15	15 (2913.45)	0	9.88/9.90	La ₂ O ₃ , Fe ₂ O ₃ , LaFeO ₃	Matured Dendrites

Note : (1) Stoichiometric ratio of 1 mM La(NO₃)₃ · xH₂O and 1 mM Fe(NO₃)₃ · 9H₂O were used for all reactions.
 (2) The reaction temperature was kept at 180 °C for 24 h.
 (3) The final products were dried at 110 °C for 1 h and calcinated at 900 °C for 3 h.
 (4) * represents the optimized final reactant concentration.

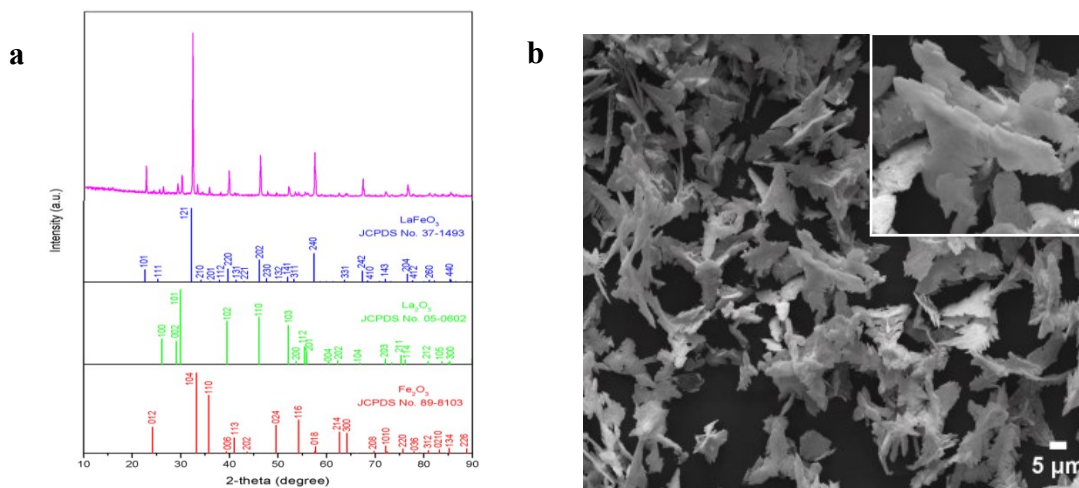


Fig. S1 a) XRD pattern and b) SEM images of 15 mM piperazine hexahydrate (P15) assisted LaFeO₃ dendrites formation process.

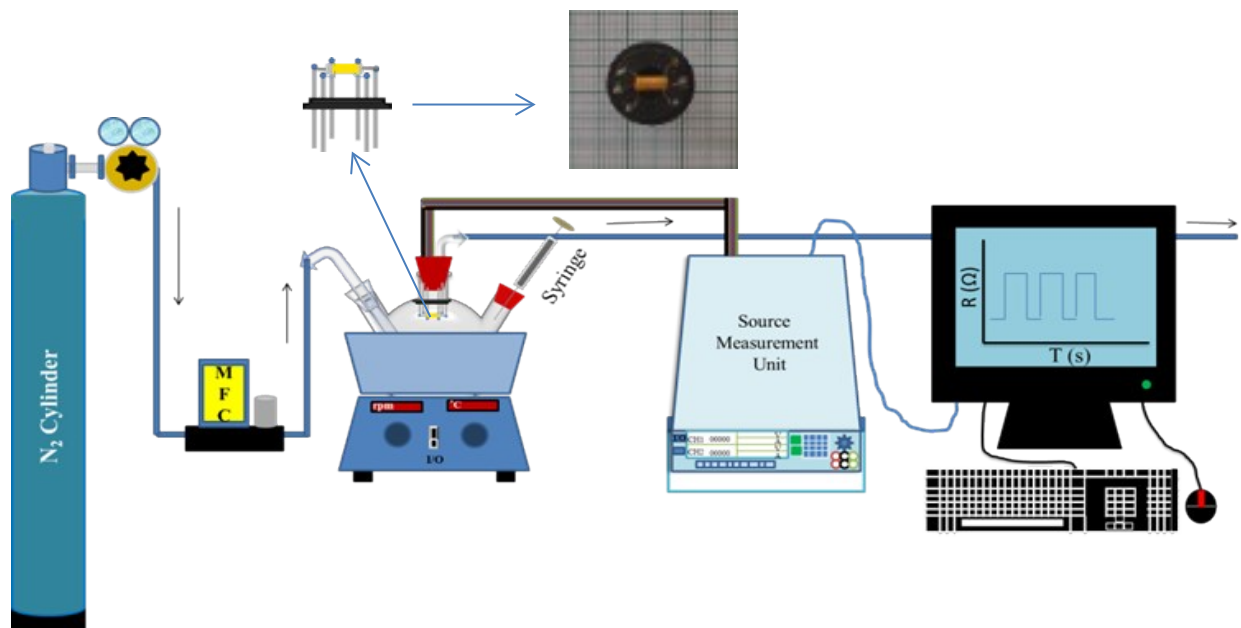


Fig. S2 Schematic illustration of custom made vapor sensing arrangement and photograph of fabricated sensing device.

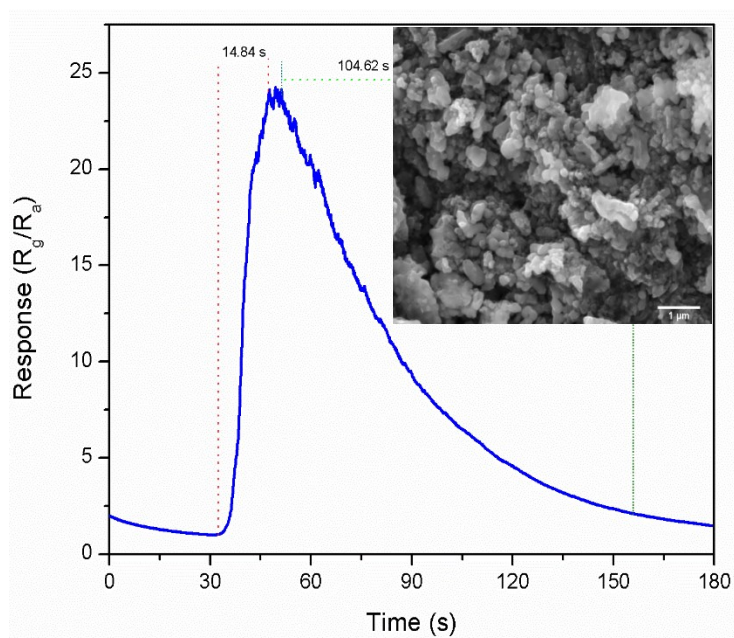


Fig. S3 1 ppm acetone sensing response using irregular LaFeO_3 particles at 100°C device and chamber temperatures. (Inset : SEM image of irregular LaFeO_3 particles)

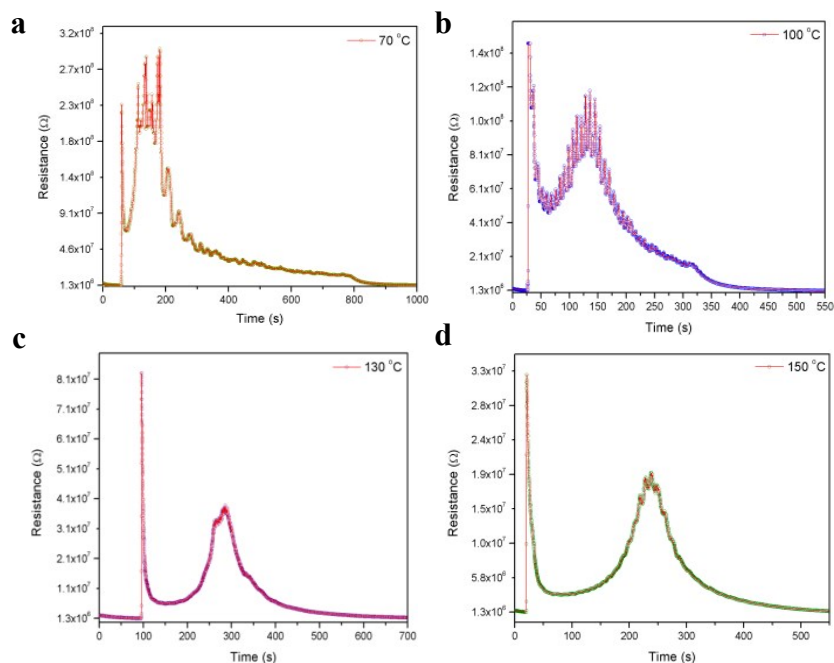


Fig. S4 10 ppm pure acetone sensing response using LaFeO₃ dendrites (U9P15) at a) 70 °C, b) 100 °C, c) 130 °C and d) 150 °C chamber temperatures with 100 °C device temperature.

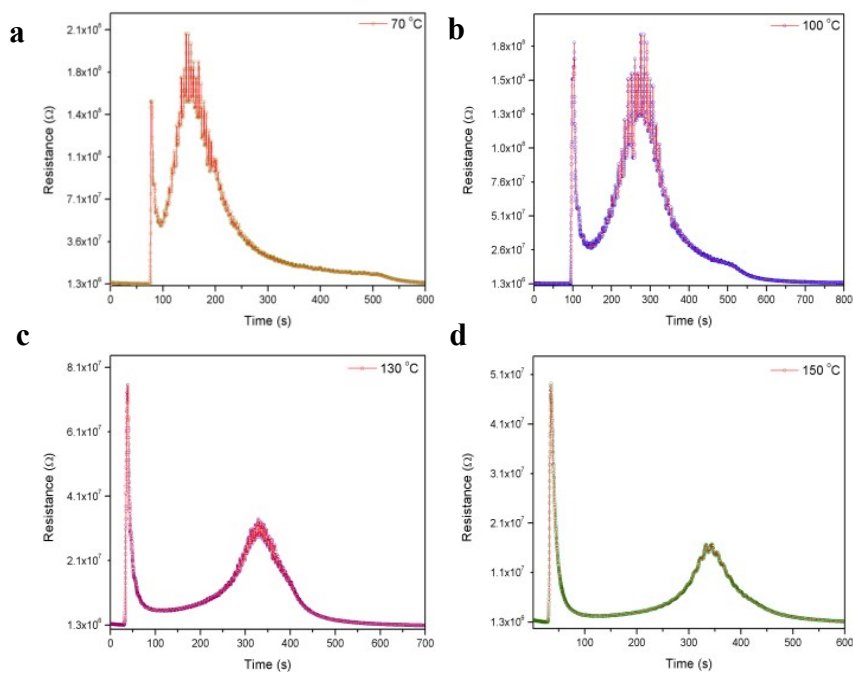


Fig. S5 10 ppm pure ethanol sensing response using LaFeO₃ dendrites (U9P15) at a) 70 °C, b) 100 °C, c) 130 °C and d) 150 °C chamber temperatures with 100 °C device temperature.

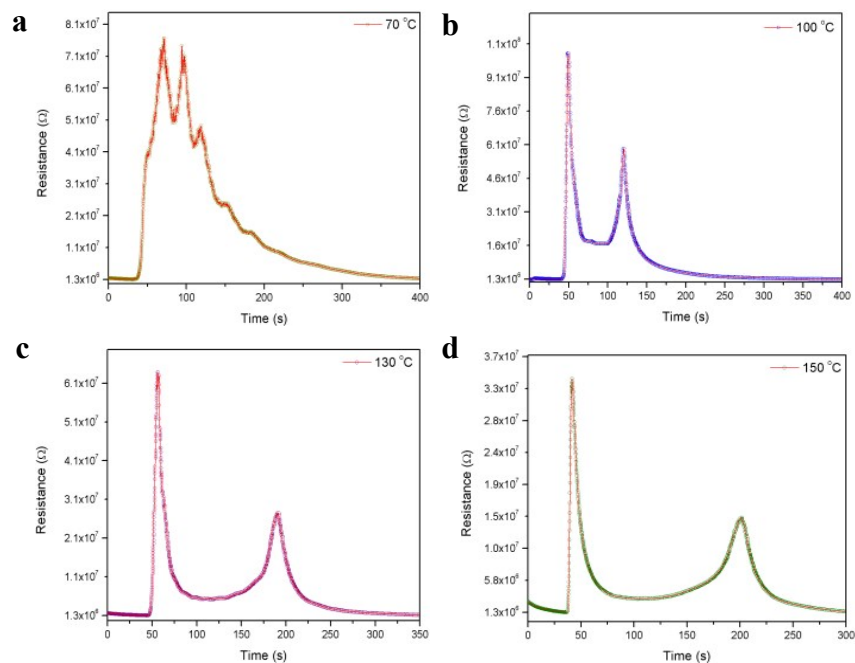


Fig. S6 10 ppm (37 - 41%) formaldehyde sensing response using LaFeO₃ dendrites (U9P15) at a) 70 °C, b) 100 °C, c) 130 °C and d) 150 °C chamber temperatures with 100 °C device temperature.

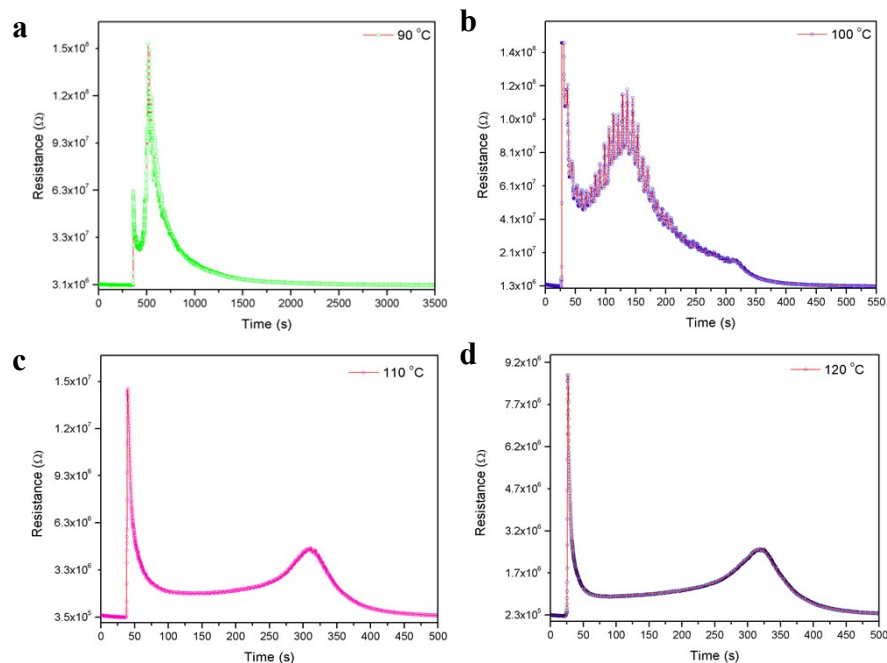


Fig. S7 10 ppm pure acetone sensing response using LaFeO₃ dendrites (U9P15) at a) 90 °C, b) 100 °C, c) 110 °C and d) 120 °C device temperatures with 100 °C chamber temperature.

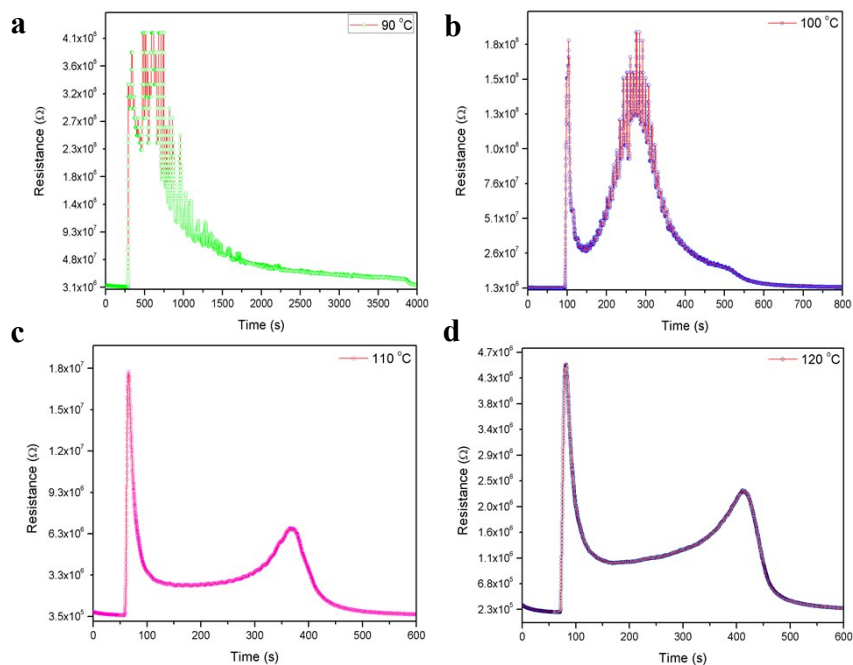


Fig. S8 10 ppm pure ethanol sensing response using LaFeO₃ dendrites (U9P15) at a) 90 °C, b) 100 °C, c) 110 °C and d) 120 °C device temperatures with 100 °C chamber temperature.

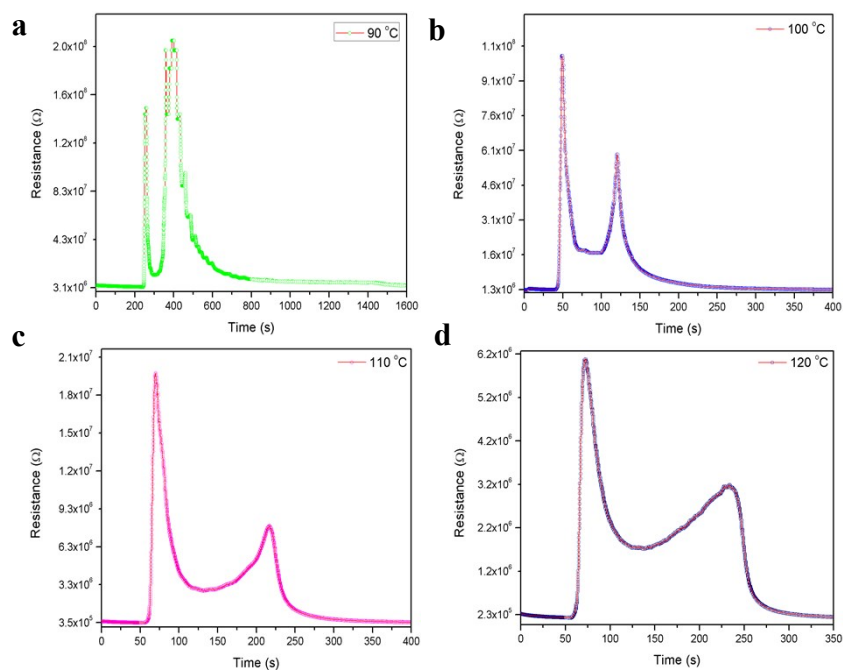


Fig. S9 10 ppm (37 - 41%) formaldehyde sensing response using LaFeO₃ dendrites (U9P15) at a) 90 °C, b) 100 °C, c) 110 °C and d) 120 °C device temperatures with 100 °C chamber temperature.

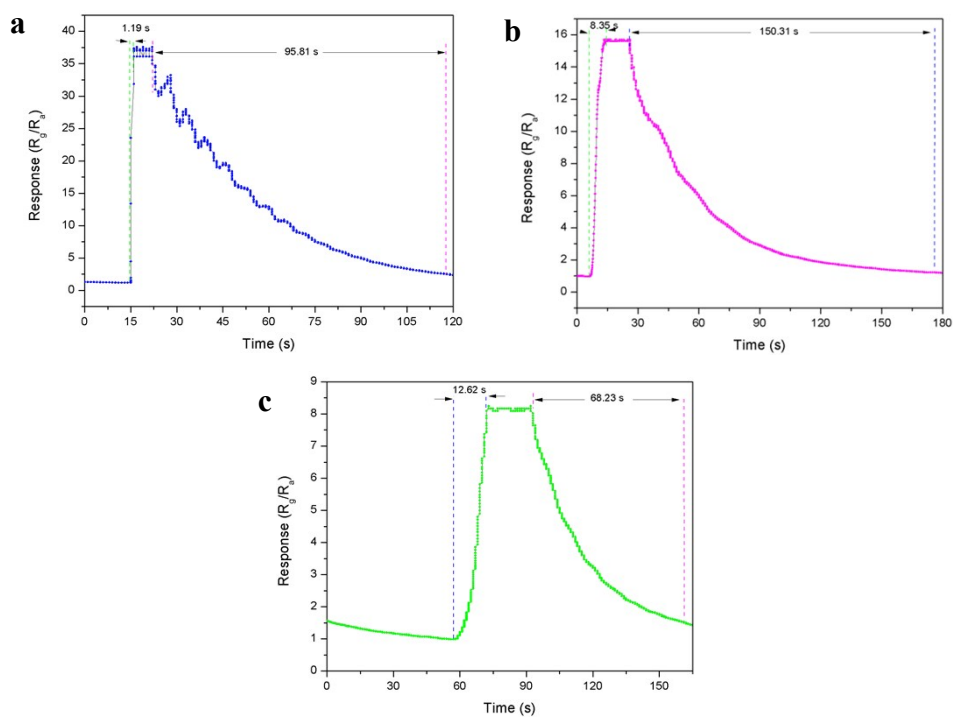


Fig. S10 Response / recovery time of 1 ppm (a) acetone, (b) ethanol and (c) formaldehyde at 100 °C device and chamber temperatures.

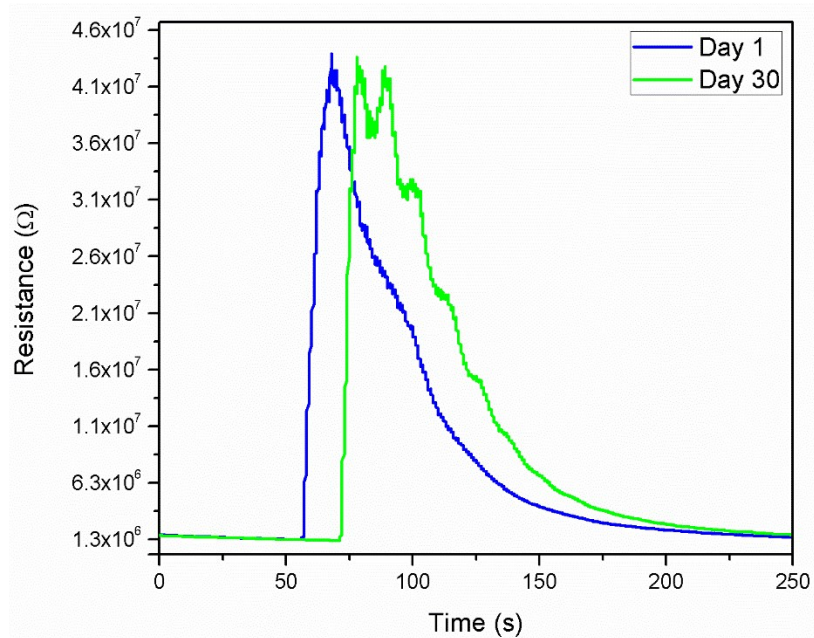


Fig. S11 Comparison of 1 ppm acetone sensing response for day 1 and day 30 using LaFeO₃ dendrites at 100 °C device and chamber temperatures.

Table S2. Comparison of recently reported acetone sensors with the present LaFeO₃ dendrites based device.

Sensing Materials	Concentration [ppm]	Sensing Response $S = R_g/R_a$ or R_a/R_g	$T_{res/rec}$ [s]	Lowest Detection [ppm]	Operating Temperature [°C]	Ref
3 mol% Co-doped Spongy-like In₂O₃	100	32.8	1.14/37.5	5	240	1
Porous WO₃ Nanofibers	12.5	1.79	33/42	1.8	350	2
3 wt% Pd:SmFe_{0.9}Mg_{0.1}O₃ Nanocrystalline Powders	0.5	7.16	32/8	0.01	220	3
Co₃O₄ Core–Shell	200	13	4/8	10	190	4
PdO–NiO/NiCo₂O₄ Truncated Nanocages	100	6.7	19/28	10	210	5
Porous Tube-like Au/ZnO	100	280	2/92	1	190	6
0.070 wt% Pt-Functionalized CS-Pt@SnO₂ Nanofiber	1	37.9	12/44	0.1	350	7
Bi₂O₃ Nanostructures	100	41%	315/152	10	27	8
Hollow NiFe₂O₄ Microspindles	200	52.8	14.2/>100	5	120	9
MWCNTs/Co₃O₄ Octahedron	100	5.1	-	10	120	10
Multilayer-assembled ZnO Nanoplates	100	21.56	9/51	0.25	230	11
Concave ZnFe₂O₄ Hollow Octahedral Nanocages	100	35.5	-	5	120	12
PdO–Co₃O₄ Hollow Nanocages	5	2.51	-	0.4	350	13
PdO–ZnO Composite on Hollow SnO₂ Nanotubes	1	5.06	16/36	0.1	400	14
PtO₂ - SnO₂ Multichannel Nanofibers	5	194.15	<12/-	0.4	400	15
γ-Fe₂O₃ Microrod	100	125.5	0.9/15	10	220	16
LaFeO₃ Dendrites	1	37.63	1.19/95.81	0.01	100	This work

References

- 1 X. Zhang, D. Song, Q. Liu, R. Chen, J. Liu, H. Zhang, J. Yu, P. Liu and J. Wang, *CrystEngComm*, 2019, **21**, 1876.
- 2 M. Imran, S. S. A. A. H. Rashi, Y. M. Sabri, N. Motta, T. Tesfamichael, P. M. Sonar and M. Shafiei, *J. Mater. Chem. C*, 2019, **7**, 2961.
- 3 H. Zhang, H. Qin, P. Zhang, and J. Hu, *ACS Appl. Mater. Interfaces*, 2018, **10**, 15558.
- 4 R. Zhang, T. Zhou, L. Wang, and T. Zhang, *ACS Appl. Mater. Interfaces*, 2018, **10**, 9765.
- 5 T. Zhou, X. Liu, R. Zhang, Y. Wang, and T. Zhang, *ACS Appl. Mater. Interfaces*, 2018, **10**, 37242.
- 6 H. Fu, X. Wang, P. Wang, Z. Wang, H. Ren and C. Wang, *Dalton Trans.*, 2018, **47**, 9014.
- 7 Y. J. Jeong, W. Koo, J. Jang, D. Kim, H. Cho and I. Kim, *Nanoscale*, 2018, **10**, 13713.
- 8 P. Shinde, B. Ghule, N. M. Shinde, Q. X. Xia, S. Shaikh, A. V. Sarode, R. S. Mane and K. H. Kim, *New J. Chem.*, 2018, **42**, 12530.
- 9 X. Song, F. Sun, S. Dai, X. Lin, K. Sun and X. Wang, *Inorg. Chem. Front.*, 2018, **5**, 1107.
- 10 R. Zhang, M. Zhang, T. Zhou and T. Zhang, *Inorg. Chem. Front.*, 2018, **5**, 2563.
- 11 M. Wang, Z. Shen, Y. Chen, Y. Zhang and H. Ji, *CrystEngComm*, 2017, **19**, 6711.
- 12 X. Z. Song, Y. L. Meng, Z. Tan, L. Qiao, T. Huang, and X. F. Wang, *Inorg. Chem.* 2017, **56**, 13646.
- 13 W. T. Koo, S. Yu, S. J. Choi, J. S. Jang, J. Y. Cheong, and I. D. Kim, *ACS Appl. Mater. Interfaces*, 2017, **9**, 8201.
- 14 W. T. Koo, J. S. Jang, S. J. Choi, H. J. Cho, and I. D. Kim, *ACS Appl. Mater. Interfaces* 2017, **9**, 18069.
- 15 Y. J. Jeong, W. T. Koo, J. S. Jang, D. H. Kim, M. H. Kim, and I. D. Kim, *ACS Appl. Mater. Interfaces*, 2018, **10**, 2016.
- 16 Z. Song, H. Chen, S. Bao, Z. Xie, Q. Kuang and L. Zheng, *J. Mater. Chem. A*, 2020, **8**, 3754.