

Supplementary Information (SI)

Graphene and Metal-Organic Frameworks Hybrids for High-Performance Sensors for Lung Cancer Biomarkers Detection supported by Machine Learning Augmentation

Trong Tuan Anh Tran^a, Kamrul Hassan^a, Tran Thanh Tung^a, Ashis Tripathy^b, Ashok Mondal^b, and Dusan Losic^a

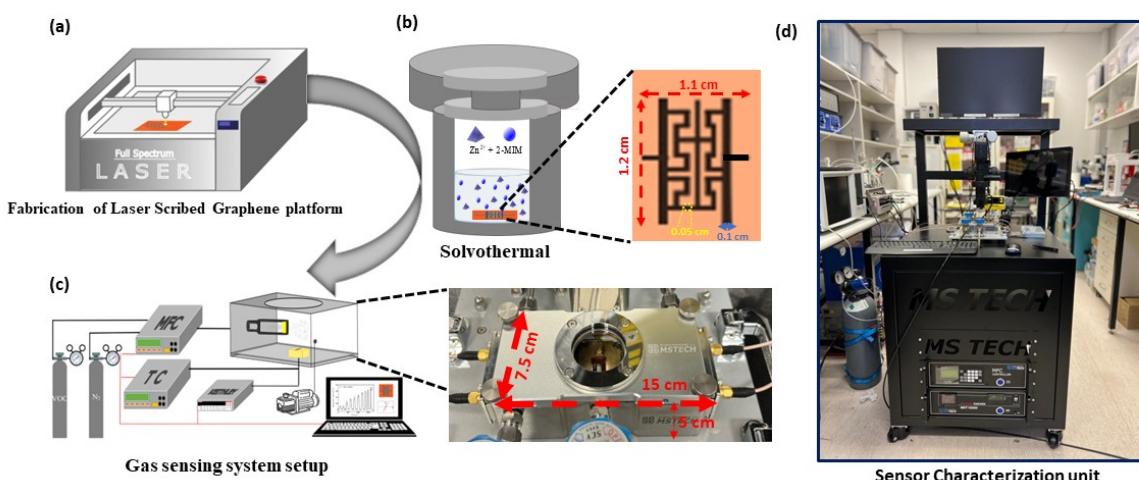


Figure S1 Schematic for ZIF-8@LSG sensor fabrication a) Laser scribing process to fabrication LSG electrode, b) Solvothermal method to grow ZIF-8 on LSG with detail size parameters of sensor, c) Gas sensing setup with detail size dimensions, d) Realistic photographic images of gas sensing set up.

Description: Figure S1 depicts the ZIF-8@LSG sensor fabrication process. To be more specific, schematic of 3 main steps to fabricate ZIF-8@LSG are illustrated in Figure S1a,b,c, which includes laser scribing step, solvothermal step and gas sensing step. Sensors was designed based on Hibert space filling design with detail size parameter showing in Figure S1b whereas the gas chamber is 7.5 cm in width, 15cm in length and 5cm in height. The full gas sensing setup is showcased in photographic images from Figure S1d.

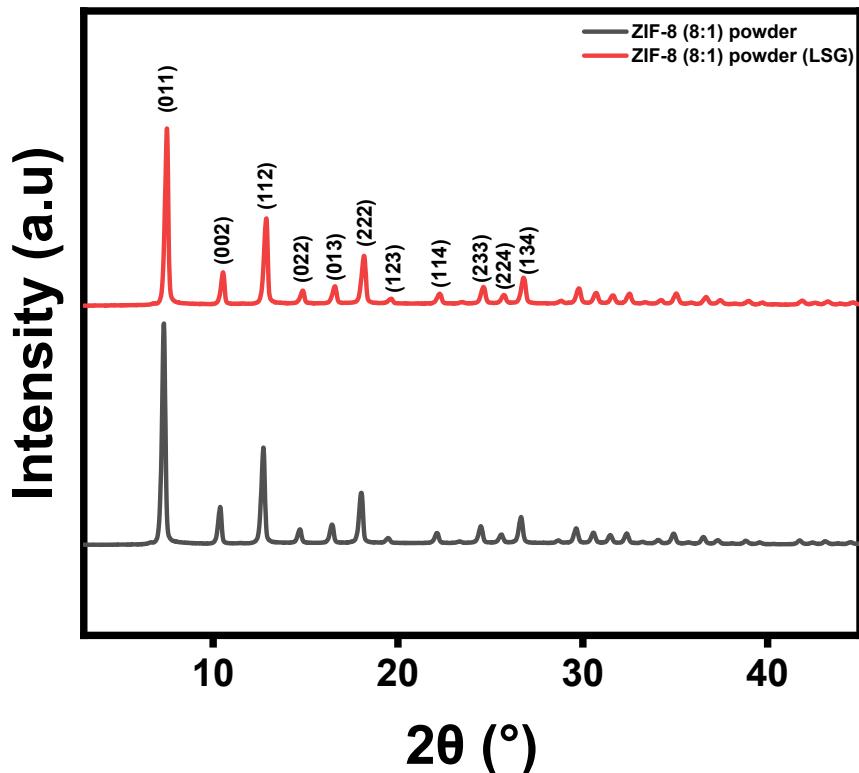


Figure S2 XRD of ZIF-8 powders

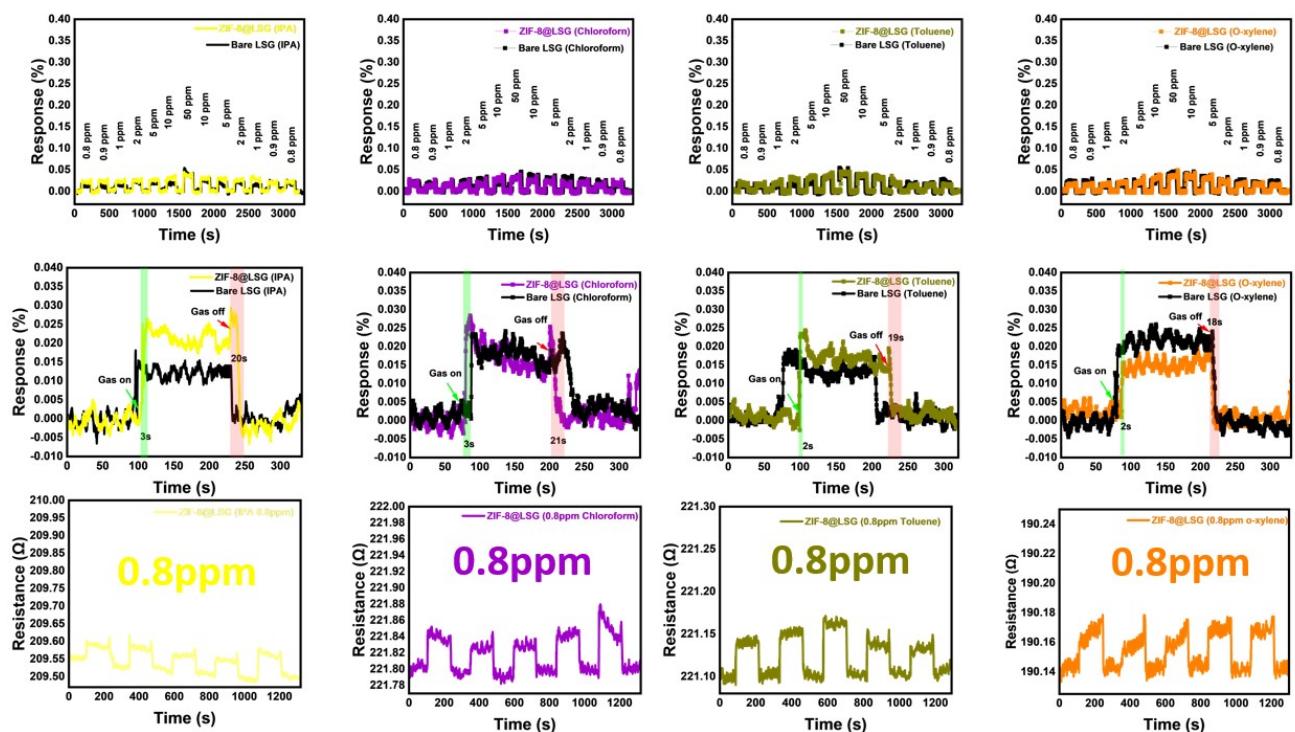


Figure S3 Sensing performance with other VOCs (IPA, Chloroform, Toluene, O-xylene)

Table T1 Linearity data of ZIF-8@LSG sensor for 8 VOCs from 0.8-10ppm

Equation	$y = a + b*x$								
	Acetone	Ethanol	Methanol	Formaldehyde	Chloroform	IPA	Toluene	o-Xylene	
Intercept (a)	0.04307 ± 0.00383	0.0741 ± 0.00357	0.06355 ± 0.00159	0.03809 ± 0.00167	0.01935 ± 0.00116	0.02376 ± 9.15683E-5	0.02104 ± 5.61306E-4	0.01884 ± 5.49216E-4	
Slope (b)	0.00985 ± 0.00103	0.00452 ± 6.4496E-4	0.00177 ± 2.58891E-4	0.00332 ± 4.51699E-4	0.00199 ± 2.99043E-4	3.30351E-4 ± 2.2982E-5	8.88798E-4 ± 6.50811E-5	0.00109 ± 1.33768E-4	
R ²	0.95815	0.92476	0.92155	0.93106	0.91692	0.98101	0.979	0.94279	

Table T2. Quantitative analysis of Biomarker classification

Biomarker	Classifier	ZIF-8@LSG (0.8-10ppm)						ZIF-8@LSG (0.8ppm)					
		SE	SP	ACC	P	R	FS	SE	SP	ACC	P	R	FS
Methanol	RBF	100	85.71	87.50	50	100	66.67	100	85.71	87.50	80	100	66.66
	MLP	100	98.41	98.50	80.51	100	89.19	100	93.75	94.53	69.56	100	82.05
O-xylene	RBF	100	85.71	87.50	50	100	66.68	36.71	94.75	87.50	50	36.7	42.34
	MLP	100	95.98	96.48	78.04	100	87.67	99.21	93.84	94.52	69.78	99.2	81.93
IPA	RBF	48.43	93.08	87.50	50	48.43	49.20	100	85.61	87.41	49.80	100	66.49
	MLP	88.28	97.65	96.48	84.32	88.28	86.25	100	93.75	94.53	69.56	100	82.05
Toluene	RBF	100	85.71	87.50	50	100	66.67	100	85.71	87.50	50	100	66.67
	MLP	100	95.98	96.48	78.05	100	87.67	100	93.75	94.53	69.56	100	82.05
Formaldehyde	RBF	51.56	92.63	87.50	50.00	51.56	50.76	100	85.71	87.50	50	100	66.66
	MLP	96.09	96.54	96.48	79.87	96.09	87.23	100	93.75	94.53	69.56	100	82.06
Ethanol	RBF	100	85.71	87.50	50	100	66.66	100	85.71	87.50	50	100	66.66
	MLP	91.40	97.20	96.48	82.39	91.40	86.67	57.03	99.88	94.53	98.64	57.0	72.27
Chloroform	RBF	100	85.71	87.50	50	100	66.67	100	85.71	87.50	50	100	66.66
	MLP	100	95.98	96.48	78.04	100	87.67	100	93.75	94.53	69.56	100	82.05
Acetone	RBF	100	85.71	87.50	50	100	66.66	63.28	90.95	87.50	50	63.2	55.86
	MLP	96.09	96.54	96.48	79.87	96.09	87.23	100	94.21	94.89	69.56	100	82.05

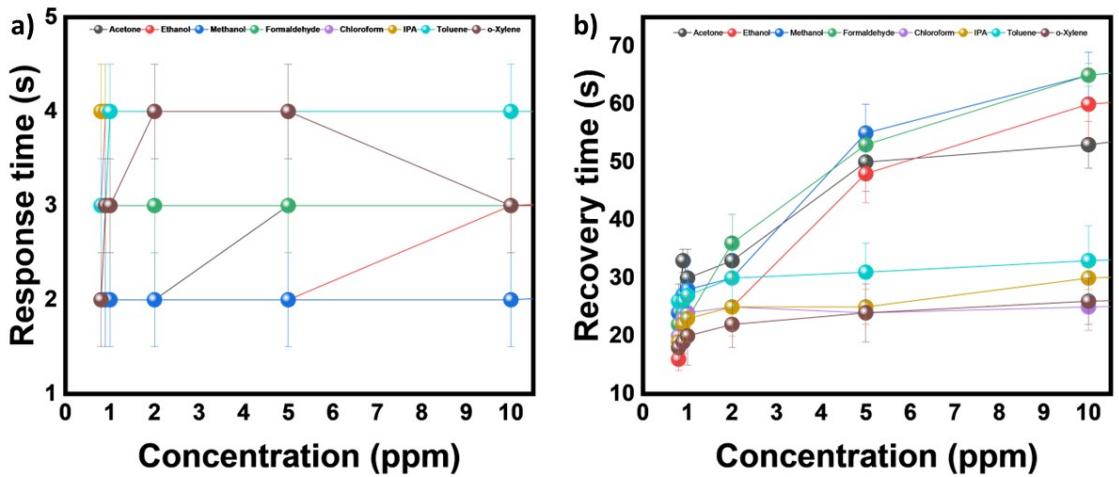


Figure S4 a) Comparative response time of ZIF-8@LSG sensor device for 8 different VOCs at different concentration; **b)** Recovery time of ZIF-8@LSG sensor device for 8 different VOCs at different concentration. (Colour code: acetone: black; ethanol: red; methanol: blue; formaldehyde: green; chloroform: purple; IPA: orange; toluene: mint blue; o-xylene: brown)

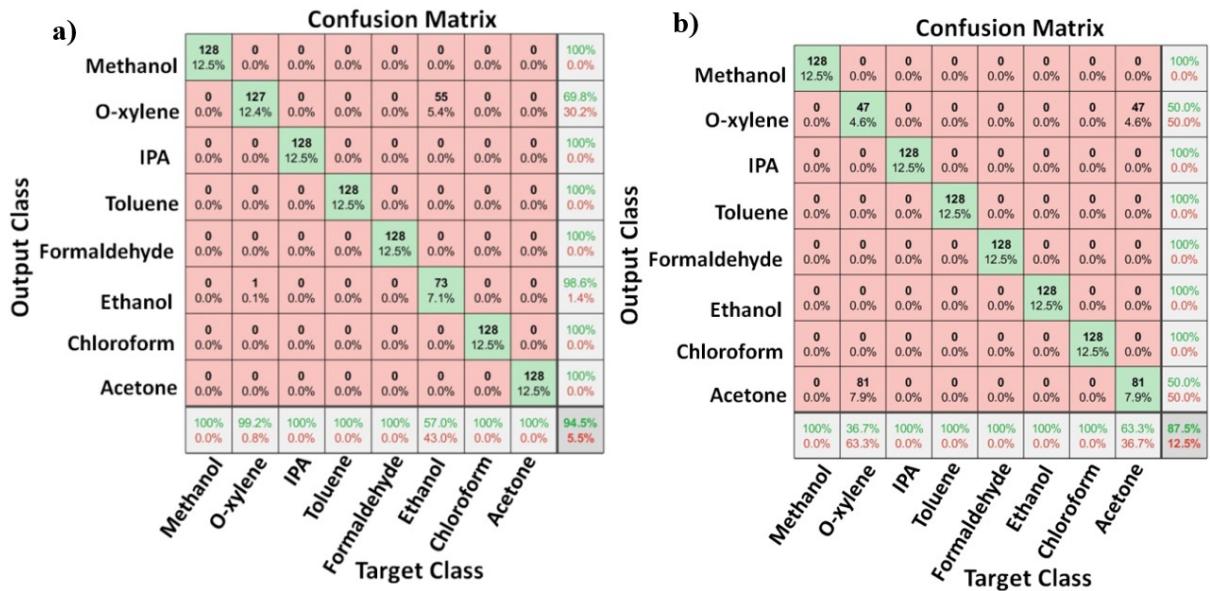


Figure S5 Graph of the test data set confusion matrix using (A) using MLP classifier algorithm for 0.8 ppm, (B) using RBF classifier algorithm for 0.8 ppm.