

# Design and Simulation of a Microcantilever Sensor for Precise Detection of Volatile Organic Compounds

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## ABSTRACT

This study presents the coating of a thin film of conducting polymer on a silicon cantilever sensor. The mechanical changes in the coated microcantilever, a bimaterial, were investigated when various volatile substances, such as methanol, ethanol, acetone, propanol, dichloroethane, and toluene were added. The results showed that the coated microcantilever is much more sensitive than the uncoated one. The maximum sensitivity observed was 40.14 kHz/ppm, demonstrating a 33.8% improvement over existing systems. Findings revealed that the maximum sensitivity achieved with the proposed sensor was 83%, and the overall improvement was 6.41%. The sensors' responses were found to be reversible, sensible, fast, and proportional to the volatile concentration.

**Keywords-**cantilever; sensor; VOC; sensitivity; MEMS; gas detection

## I. INTRODUCTION

The detection of various vapors plays an important role in sensor technology. The microcantilever is a widely used component in microsystem devices that has turned out to be an outstanding platform for various sensitive sensors in recent years. The rigid end of a cantilever applies stress to the free end. A microcantilever serves as a physical, chemical, or biological sensor by detecting changes in cantilever bending or vibration frequency. Microcantilevers have become popular over the past few decades due to their high sensitivity, selectivity, ease of fabrication, and flexibility in on-chip circuits. Due to its convenience in regulating and being readily adjustable into a unified electromechanical system, it provides a wide range of industrial applications [1]. These sensors consist of a receptor that is specialized for a specific chemical or biological target to monitor the resonant frequency, which shifts due to the mass attached to the structure. The amount of

attached mass or any other type of force acting upon it correlates with the difference in resonance frequency. Microcantilever sensors can be used in air, vacuum, or liquid. However, the damping effect in a liquid medium reduces the microcantilever's resonance response, whereas the bending response remains the same in a liquid medium. As a result, the practicality of operating a microcantilever in a solution with high sensitivity makes it an ideal platform for chemical sensors and biosensors. These cantilever sensors provide better dynamic response, reduced size, high accuracy, and increased reliability than common sensors [2].

This paper considers the Finite Element Method (FEM) and how it can be utilized to make a microcantilever sensor work accurately for methanol, ethanol, acetone, propanol, dichloroethane, and toluene, among other Volatile Organic Compounds (VOCs). Analytical calculations and simulations for a nonlinear array cantilever have been carried out by using

the FEM. A model of the cantilever beams was developed and the chemical module was utilized employing COMSOL Multiphysics to design chemical pillars for the vapor analysis.

The adsorption of analytes onto the detecting surface of the microcantilever sensor is the fundamental mechanism behind the way this kind of sensor works. The adsorption of analytes onto the sensing surface, which causes a differential surface tension and increases the microcantilever's mass is the basis for the operation of the microcantilever sensor. The functionalized surfaces of the microcantilevers make them excellent for selectively detecting small quantities of chemicals. In addition, these sensors are capable of detecting physical, chemical, or biological stimuli, and they offer many benefits over conventional approaches, such as high sensitivity, inexpensiveness, simple operation, and rapid responses. Therefore, a variety of industries, including safety and security, environmental monitoring, and food, have the potential to use the sensor [3-5].

TABLE I. VOC ANALYTES AND REACTANTS

Analyte	Chemical formula	Surface reactants
Methanol	CH <sub>3</sub> OH	Trimethoxymethylsilane (TMMS)
Ethanol	C <sub>2</sub> H <sub>5</sub> OH	Trimethyl silane (TMS)
Acetone	CH <sub>3</sub> C <sub>2</sub> OH	Organ silanes with ketone-specific ligands
Propanol	C <sub>3</sub> H <sub>7</sub> OH	Propyl group-modified silane coupling agents
Dichloro ethane	C <sub>2</sub> H <sub>2</sub> C <sub>12</sub>	Chlorinated compound-interacting polymers
Toluene	C <sub>7</sub> H <sub>8</sub>	Carbon nanotubes, graphene, porous polymers

## II. LITERATURE SURVEY

One method of vapor detection is the quartz crystal microbalance in which alkane thiols form monolayers over the quartz crystal microbalance [6, 7]. The organic vapors interact with monolayers via hydrogen bonding and dipole interaction, resulting in mass changes. Another method involves coating a cantilever with arsenic adsorbent, based on a piezoresistive arsenic sensor [8, 9]. As a result, when the sensing cantilever interacts with arsenic particles, its resistance changes.

In [10-13] various cantilever beam structures were analyzed to determine the most suitable one. The different beams were subject to the same mechanical force and the corresponding displacements and eigenfrequencies were analyzed. The most commonly used high-accuracy methods are optical reflection,

piezoresistive, capacitance, and piezoelectric. The advantage of implementing these techniques is that both frequency and bending can be measured in a single measurement [14, 15]. This allows them to estimate and detect VOCs, which are compounds that vaporize at ambient temperature and pressure, with greater precision [16–18]. Table II demonstrates the related literature survey.

## III. MATHEMATICAL ANALYSIS AND MODELING

The newly designed MEMS cantilever sensor works on the assumption that the target gas is dispersed evenly throughout the cantilever surface and exerts only a small force. The distribution of the target gas exerts the force on the sensor surface.

$$F = ma \quad (1)$$

Cantilever structures are governed by a generic governing equation [17], which is denoted by:

$$-EI \frac{\partial^2 w}{\partial v^2} = Fv - m_o - \int_0^v \frac{F}{l} (v - s) \partial s \quad (2)$$

where E is the modulus of elasticity, I is the moment of Inertia or rotational inertia,  $\frac{\partial^2 w}{\partial v^2}$  is the second order derivation of the deflection, F is the uniform force delivered as a result of surface deformation when the target gas interacts with the sensor surface, v is the location of origin, m<sub>o</sub> is the moment of hinges, and s is the point where the interaction between the target gas and the coated material occurs.

By integrating (2) with respect to s it is obtained:

$$-EI \frac{\partial^2 w}{\partial v^2} = Fv - m_o - \frac{F}{l} \left( vs - \frac{s^2}{2} \right) \text{Lim } 0 \text{ to } v \quad (3)$$

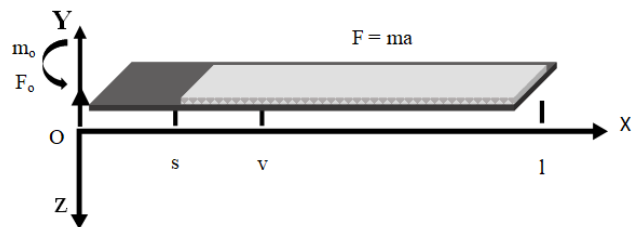


Fig. 1. Cantilever load with a consistent distribution of the expected target gas.

TABLE II. LITERATURE SURVEY

Objective	Methodology	Analyte	Sensitivity (%)	Key Findings	Limitations	Ref.
Detect methylalcohol using a chemo sensor	Chemo sensor-Micromechanical	Methyl alcohol	86.74	Achieved high sensitivity for methylalcohol detection	Limited to methylalcohol detection	[18]
Detect acetone using MEMS technology	MEMS Piezoresistive Cantilever	Acetone	77.40	Achieved good sensitivity for acetone detection	Focuses only on acetone	[17]
Multi-analyte detection	MEMS Microcantilever	Acetone, ethanol	75.8 and 80.2	Achieved reasonable sensitivity for acetone detection	Limited to acetone and ethanol	[19]
Detect benzene using MEMS technology	MEMS PZT Cantilever	Benzene	75.9	Achieved good sensitivity for benzene detection	Only evaluates benzene	[20]
Multi-analyte detection	MEMS Microcantilever	Acetone, benzene, ethanol, toluene	78.56, 79.56, 79.58, 84.56	Achieved high sensitivity for acetone detection	Lack of selectivity among similar analytes	[21]

Applying limits and performing simple calculations to (3) we get:

$$-EI \frac{\partial^2 w}{\partial v^2} = Fv - m_o - \frac{F}{1} \left( v^2 - \frac{v^2}{2} \right) \tag{4}$$

$$-EI \frac{\partial^2 w}{\partial v^2} = Fv - m_o - \frac{F v^2}{1} \tag{5}$$

$$\frac{\partial^2 w}{\partial v^2} = \left[ \frac{Fv^2}{21} + m_o - Fv \right] \frac{1}{EI} \tag{6}$$

The stress S(v) formed on surface cantilever is given by:

$$S(v) = -E \left( \frac{-k}{2} \right) \frac{\partial^2 w}{\partial v^2} \tag{7}$$

where k is the cantilever beam thickness. By plugging (6) into (7), we are able to calculate the stress that accumulates on the cantilever as a result of the reaction that takes place among the gas of interest and the coating substance at point s.

$$S(v) = -E \left( \frac{-K}{2} \right) \left[ \frac{Fv^2}{21} + m_o - Fv \right] \frac{1}{EI} \tag{8}$$

By applying the boundary conditions  $v = 1$  and  $\frac{\partial^2 w}{\partial v^2} (\text{Lim } l = 0)$  in (5), we get:

$$-EI \frac{\partial^2 w}{\partial v^2} = Fl - m_o - \frac{Fl^2}{21} \tag{9}$$

The value of  $m_o$  is given by:

$$m_o = \frac{Fl}{2} \tag{10}$$

Substituting  $m_o$  in (8) leads to:

$$S(v) = -E \left( \frac{-K}{2} \right) \left[ \frac{Fv^2}{21} + \frac{Fl}{2} \right] \frac{1}{EI} \tag{11}$$

$$S(v) = \left( \frac{K}{21} \right) \left[ \frac{Fv^2}{21} + \frac{Fl}{2} - Fv \right] \tag{12}$$

Simplifying (12) we get:

$$S(v) = \frac{K}{41l} (Fl^2 + Fv^2 - 2Fvl) \tag{13}$$

The maximum force on the cantilever is calculated by plugging  $v=0$  into (13):

$$S(v)_{\max} = \frac{K}{41l} Fl^2 \tag{14}$$

By substituting  $l = \frac{41BK^3}{12}$  we get:

$$S(v)_{\max} = \frac{K}{41BK^3} Fl \tag{15}$$

$$S(v)_{\max} = \frac{3}{bk^2} Fl \tag{16}$$

By inserting (1) into (16), one can determine the maximum stress,  $S(v)_{\max}$ , on the cantilever that is caused by the interaction between the exposed gas and the coated material.

$$S(v)_{\max} = \frac{3ml^2}{k^2} \tag{17}$$

where F is the force of deflection that is produced as a result of surface deformation, m is the mass created by the exposed gas, and A is the surface area.

For cantilever construction, the transverse and longitudinal modes of operation are taken into consideration in this modeling. The designed cantilever sensor operates transversely in this investigation. Equation (18) describes contact pads resistance.

$$R(v) = L S(v)t \tag{18}$$

where L is the coefficient of resistance of the coating material, R(v) is the induced resistance, and S(v) is the stress.

The conventional definition of sensitivity is calculated by:

$$\text{Sensitivity} = \frac{\Delta \text{Output}}{\Delta \text{Input}} = \frac{\Delta R}{\Delta F} = \frac{R}{ma} \tag{19}$$

The strain applied to the cantilever is one way to convey sensitivity:

$$\text{Sensitivity} = \frac{L t (S(v)2 - S(v)1)}{m2 - m1} \tag{20}$$

where L is the coating material's coefficient of resistance, S(v)2 is the measured strain on the cantilever's surface after the detection of the target gas at a  $v = 2$ , S(v) 1 is the surface stress at  $v = 0$ , m2 is the mass of the cantilever at  $v = 1$ , and m1 is the mass of the cantilever at  $v = 0$ .

Based on (17), it would be reasonable to come to the conclusion that the sensitivity and length are directly proportional to each other, and the dependence on thickness is exactly inversely proportional to it, or k. Sensitivity is determined by mathematical equations that take into account the length of the cantilever and the thickness of the coating. This provides parameters for sensor modeling, illustrating their sensitivity and the impact of other sensors involved in the process. The next section describes an experimental procedure that aims to determine the cantilever's response to the targeted gas.

#### IV. MATERIALS AND METHODS

Utilizing COMSOL Multiphysics for simulating the behavior of a non-linear array of MEMS microcantilevers for VOC detection requires a multi-disciplinary approach encompassing mechanical, chemical, and electrical engineering principles along with computational modeling techniques. Adjustments to the methodology might be necessary based on specific VOCs, sensor characteristics, and desired detection capabilities. This research made use of commercially available rectangular silicon microcantilevers. The dimensions of these microcantilevers are shown in Table III.

TABLE III. ARRAY CANTILEVER DIMENSIONS

Particulars	Dimensions
Total array width	172.5um
Beam thickness	0.5um
Support beam width	22.5um
Spacing	21.5um
Beam 1 (CL-6)	45um×12.5um×0.5um
Beam 2 (CL-5)	50um×12.5um×0.5um
Beam 3 (CL-4)	55um×12.5um×0.5um
Beam 4 (CL-3)	60um×12.5um×0.5um
Beam 5 (CL-2)	65um×12.5um×0.5um
Beam 6 (CL-1)	70um×12.5um×0.5um

The sensor's response was evaluated to a variety of VOCs in a simulation environment, using a range of VOC concentrations from 0 to 1000 ppm. We arranged the sensor's exposure to volatiles by polarity (from polar to nonpolar) at 0, 100, 250, 500, 750, and 1000 ppm. This was done because nonpolar chemicals could damage the sensitive layer and make the sensor to not work properly. We employed methanol, ethanol, acetone, propanol, dichloroethane, and toluene as the volatile substances. Despite being liquids, all the examined VOC vaporized readily at room temperature and pressure. We measured the amount of deflection each encountered in terms of resonance frequency to examine the sensitivity of the coated and uncoated microcantilevers. Table IV displays the material characteristics of the proposed array cantilever.

TABLE IV. PROPERTIES USED TO SIMULATE THE CANTILEVER ARRAY

Parameter	Symbol	Value	Units
Young modulus	E	180	Gpa
Density	P	2300	Kg/m <sup>3</sup>
Poisson ratio	N	0.28	-

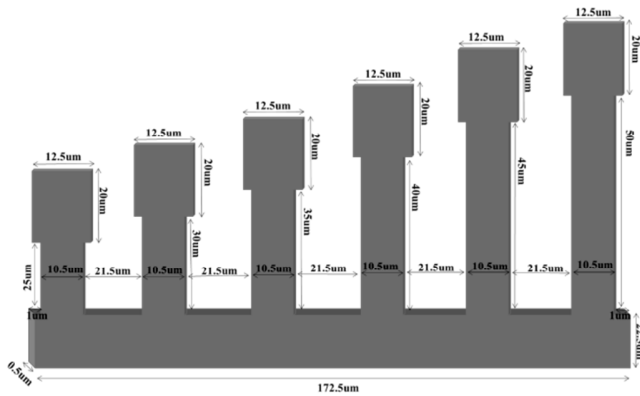


Fig. 2. Structural dimensions of the proposed nonlinear cantilever array.

In COMSOL, the fine mesh analysis shown in Figure 3 entails modifying the computational grid to capture subtle features in simulations. Adjusting mesh size, element styles, and mesh control in key areas improves accuracy, particularly for MEMS microcantilever models that detect VOCs. Mesh refinement studies evaluate convergence and solution accuracy to achieve the best balance of computational efficiency and result precision.

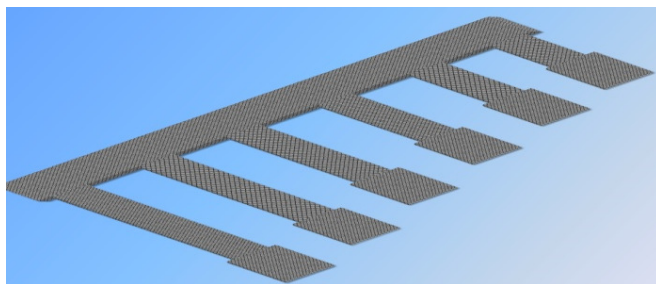


Fig. 3. Super fine mesh analysis.

## V. RESULTS AND DISCUSSION

Figure 4 shows the deflections of the different cantilever for the respective forces. Here, the beams are of the same material (Si) which has the best properties suitable for chemical vapor detection. Figure 4 shows the mass loading of a rectangular micro cantilever beam for the respective mass which shows the maximum deflection at the eigenfrequency

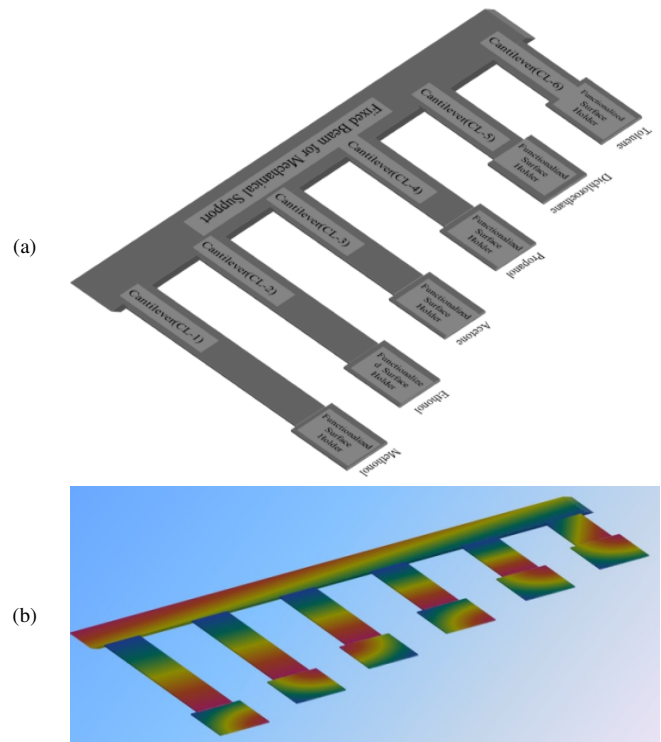


Fig. 4. (a) Cantilever specific coating, (b) developed cantilever in COMSOL simulator.

Figure 4(a) shows specific VOC assignments and Figure 4(b) shows the designed cantilever array. In the non-functionalized state, the frequencies range from 125.98 kHz to 137.84 kHz, with displacements between 27.86 nm and 52.34 nm. This indicates the baseline mechanical properties of the cantilevers without any modifications or external influences.

Figure 5 reveals a significant decrease in frequencies, from 106.72 kHz to 119.85 kHz, upon full functionalization with a reactant coat. The displacements also show variations, with the highest value at 61.32 nm for CL-1 and the lowest at 29.96 nm for CL-6. The decrease in frequency suggests that the added mass from the reactant coat influences the mechanical properties of the cantilevers, increasing their mass and reducing their stiffness.

Table V shows information about the natural frequency response of a microcantilever array when it is not functionalized, fully functionalized with a reactant coat, and exposed to a certain VOC. Each condition's frequency ( $f_0$ ) in kHz and displacement ( $\delta$ ) in nm are recorded for six cantilevers (CL-1 to CL-6).

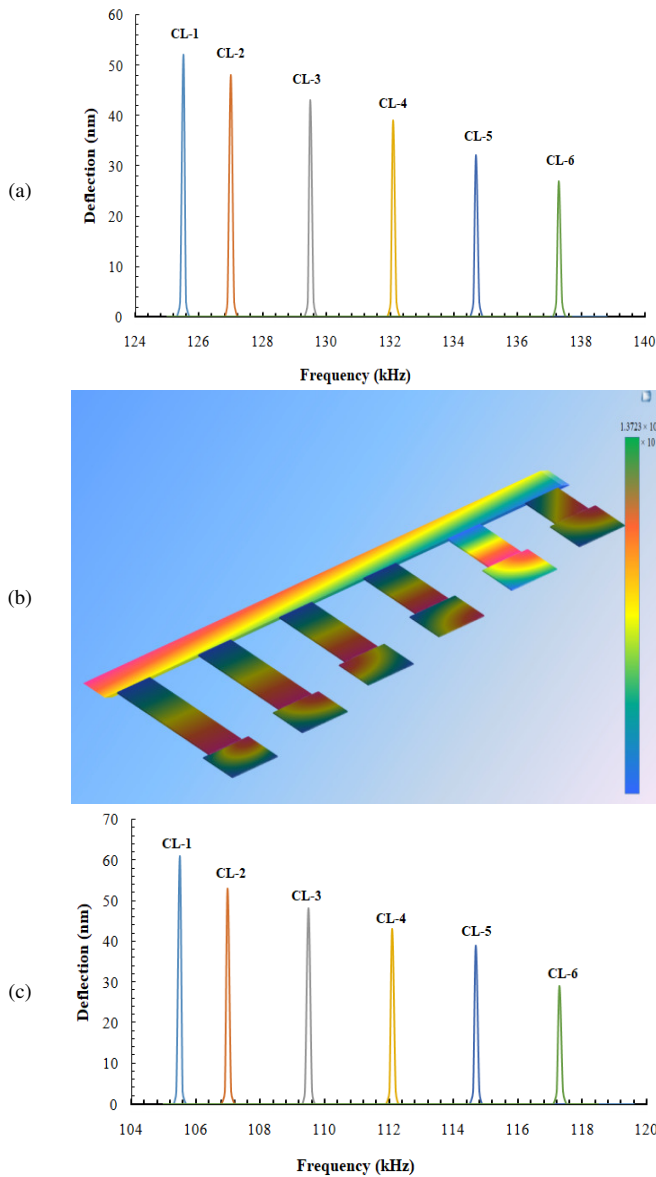


Fig. 5. Change in resonance performance: (a) Cantilever under non-functionalization, (b) simulation analysis for functionalization, (c) change in the resonance response under functionalization.

TABLE V. FREQUENCY RESPONSE OF THE CANTILEVER ARRAY

CL	NFC		FFC		ESV	
	$f_o$ (kHz)	$\delta$ (nm)	$f_o$ (kHz)	$\delta$ (nm)	$f_o$ (kHz)	$\delta$ (nm)
CL-1	125.98	52.34	105.72	61.32	86.84	128.95
CL-2	127.78	48.48	107.37	53.36	89.78	126.45
CL-3	129.56	43.56	109.89	48.46	92.24	124.65
CL-4	132.42	39.15	112.54	43.96	94.56	119.89
CL-5	135.03	32.31	115.64	39.82	97.34	116.78
CL-6	137.84	27.86	117.85	29.96	99.43	112.62

\*CL - Cantilever, \*NFC - Non-Functionalized Cantiliver, \*FFC- Fully Functionalized Cantilever  
\*ESV-Exposed Specific VOC

Upon exposure to a specific VOC, the frequencies further decrease for each cantilever, ranging from 86.84 kHz to 99.43 kHz. This further decrease in frequency and increase in

displacement indicate a significant interaction between the VOC and the coated cantilevers, likely due to the adsorption or chemical interaction, which adds mass or alters the surface properties.

Table V shows how sensitive microcantilevers are to changes in surface and environmental exposure. This shows that they could be used in sensing applications where changes in frequency and displacement can show that certain substances are present.

Table VI shows the comparison between the theoretical and the simulation results for the natural frequency ( $f_o$ ) in kHz and displacement ( $\delta$ ) in nm. The frequencies range theoretically from 84.56 kHz to 97.85 kHz, and in simulations from 86.84 kHz to 99.43 kHz. Displacement ranges from 113.89 nm to 132.54 nm theoretically and 112.62 nm to 128.95 nm in simulations. The percentage differences between theoretical and simulation frequencies range from 2.64% to 2.75%, while the displacement differences range from 1.12% to 3.97%. This indicates that simulation results closely match the theoretical predictions, validating the simulation model's accuracy.

TABLE VI. COMPARISON BETWEEN THEORICAL AND SIMULATIONAL RESULTS

Theoretical analysis		Simulation results	
$f_o$ (kHz)	$\delta$ (nm)	$f_o$ (kHz)	$\delta$ (nm)
84.56	132.54	86.84	128.95
87.87	129.83	89.78	126.45
89.45	128.67	92.24	124.65
91.34	124.86	94.56	119.89
94.98	113.89	97.34	116.78
97.85	118.37	99.43	112.62

Average sensitivity calculation for each case:

Calculate the average sensitivity for non-functionalized, fully functionalized, and specific VOC conditions.

$$S_{avg} = \sum_{i=1}^6 S_i / 6 \tag{21}$$

To calculate the percentage sensitivity of the proposed system (22) is applied:

$$\% \text{ of Improvement} = \frac{S_{proposed} - S_{Existing}}{S_{Existing}} \times 100 \tag{22}$$

TABLE VII. SENSITIVITY OF CANTILEVER SENSOR ARRAY

Cantilever	Analyte	Sensitivity
CL-1	Methanol	84.76
CL-2	Ethanol	83.58
CL-3	Acetone	86.56
CL-4	Propanol	83.50
CL-5	Dichloroethane	79.30
CL-6	Toluene	81.30

The average sensitivity of the proposed sensor is approximately 83%. Compared to similar multi-analyte detection sensors from [19], the proposed sensor shows a 6.41% improvement in overall sensitivity.

## VI. CONCLUSION

A silicon cantilever sensor coated with a conducting polymer film was investigated for detecting various Volatile

Organic Compounds (VOCs), including methanol, ethanol, acetone, propanol, dichloroethane, and toluene. We measured the mechanical deflection responses of both coated and uncoated microcantilevers. The results demonstrated that the coated microcantilever exhibited significantly higher sensitivity compared to the uncoated one. The sensitivity was directly proportional to the VOC concentration, and the specific reactant coat on the cantilever surface significantly improved the sensor sensitivity by 6.14% compared with the existing and the overall sensitivity of the proposed sensor was 83%.

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