Statistical analysis for selective identifications of VOCs by using surface functionalized MoS_2 based sensor array

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Outline

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Introduction

- Breath analysis gained a lot of interest for the non-invasive detection of diseases and monitoring health parameters.
- More than 1000 volatile organic components (VOCs) are present in the exhaled breath, only some of them are considered as diseases markers.
- The combination of a highly selective sensors and an effective machine learning can be used for early detection of diseases.
- Chemiresistive sensors is suitable for recognizing the target VOCs.
- Pattern recognition algorithms like k-nearest neighbor, Discriminant Function Analysis, support vector machine, random forest, logistic regression, etc. plays an essential role for classification of VOCs

Material and Methods

- **Preparation of MoS_2**

- **Sensor Fabrication**

Preparation of MoS_2

- All materials MoS_2 (Sigma Aldrich), gold (III) chloride ($AuCl_3$, 99 %, Sigma Aldrich), palladium chloride ($PdCl_2$, 60%, Molychem) and chloroplatinic acid ($H_4PtCl_6xH_2O$, 40 %, Molychem) were analytical grade and used without further any purification. 0.2 Wt% MoS_2 solution was prepared in deionized water and stirred for 1.5 h at room temperature to maintain homogeneity.
- Au, Pd and Pt nanoparticle loaded MoS_2 samples were prepared by spray coating technique. Firstly, MoS_2 solution was spray coated on washed SiO_2/Si substrate and dried at room temperature.
- A thermal annealing was performed for 4 h at 250 ˚C to provide crystallization and thermal stability in all 4 samples (MoS_2, Au-MOS_2, Pd-MoS_2 and Pt-MoS_2).

Fabrication of Sensor

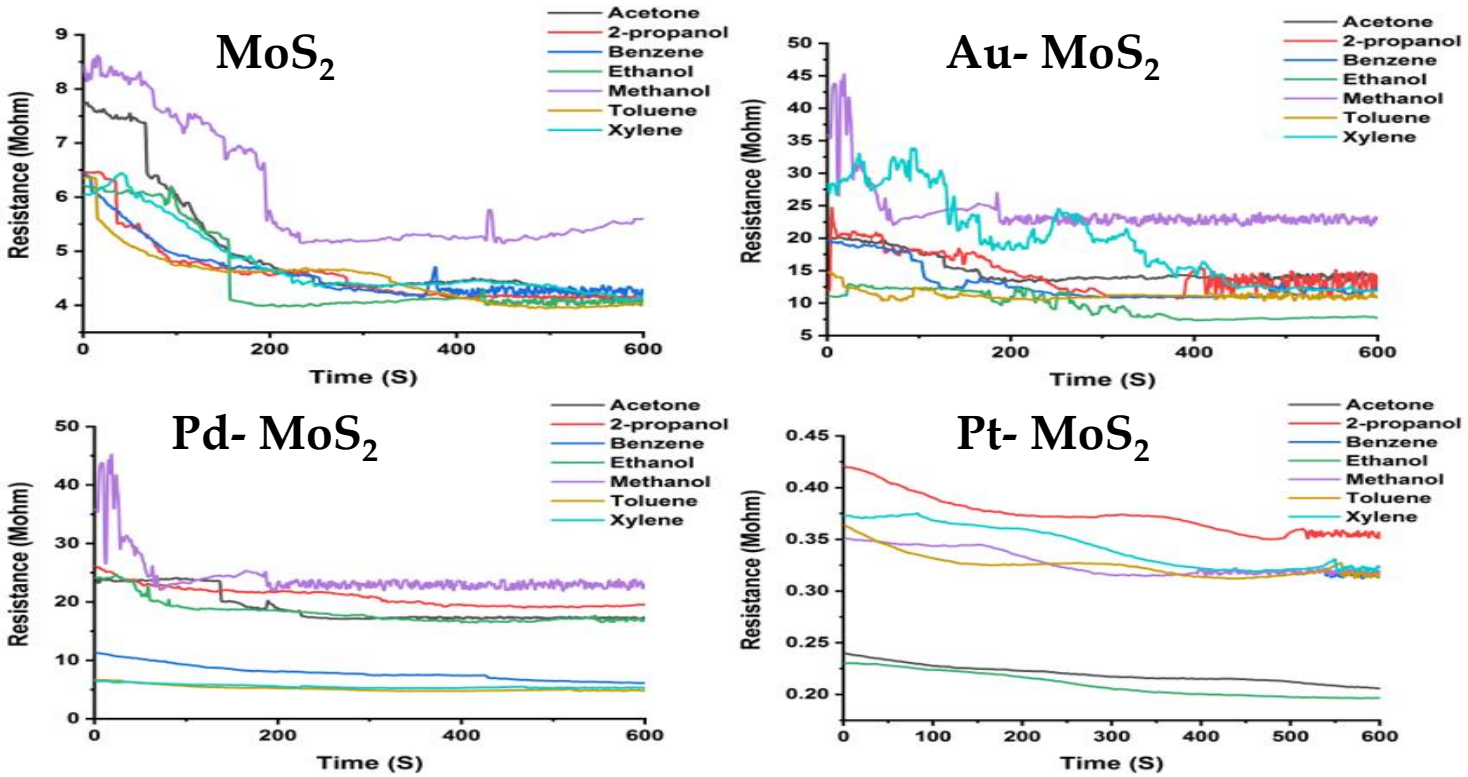
- Au source and drain electrodes of 150 nm thickness were deposited on all four samples by using electron bean evaporation unit.
- Sensors was then placed into a sensor holder and further sensing performance was studied.
- The sensing performance of prepared sensors was examined by static mode sensing setup where, VOCs were injected by using micro syringes (Hamilton micro syringe) and sensor was recovered by flowing 450 SCCM synthetic air by using mass flow controller.

Results and Discussion

- VOC Sensing
- Data Analysis
- VOC Identification

VOC Sensing

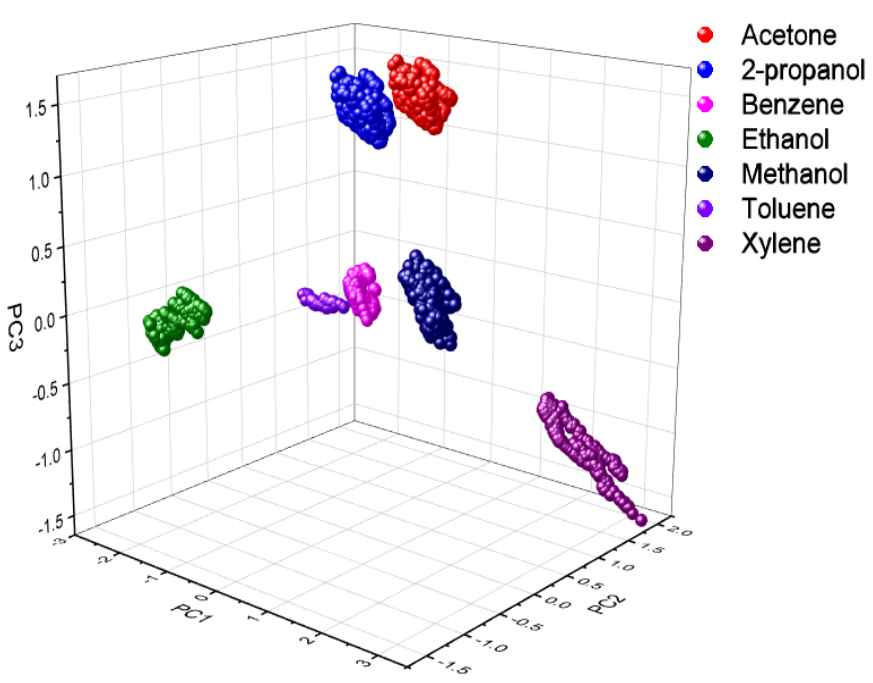
- Synthetic air was used to perform the gas sensing measurements of four different sensors: pure MoS_2, Au- MoS_2, Pd- MoS_2 and Pt- MoS_2

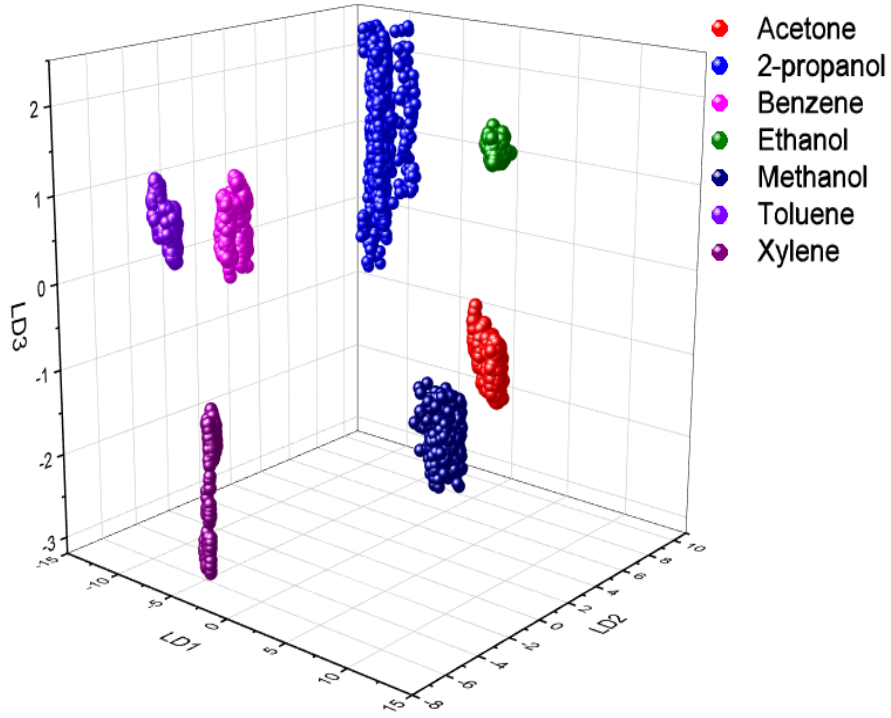


Data Analysis

- The four different sensors for seven different VOCs was used for principal component analysis (PCA).
- LDA was also performed on the same data which was used for PCA

PCA and LDA Output



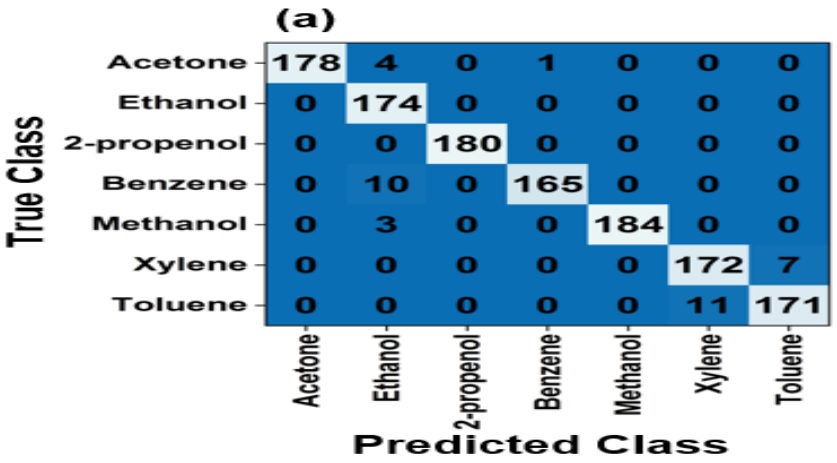


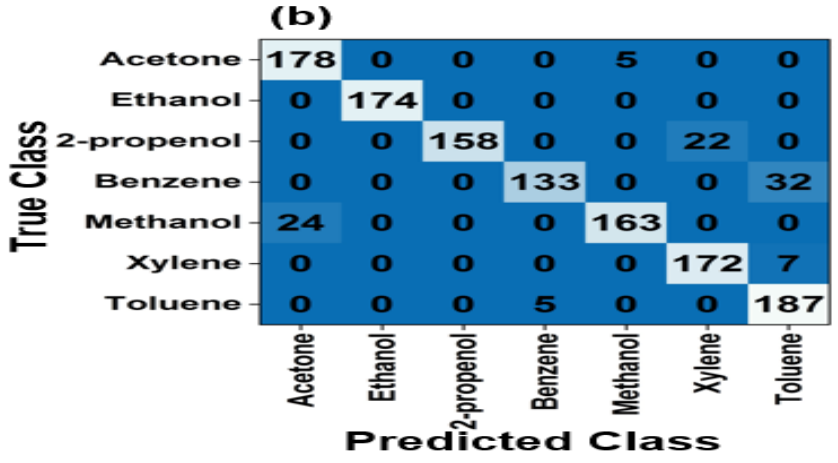
VOC Identification

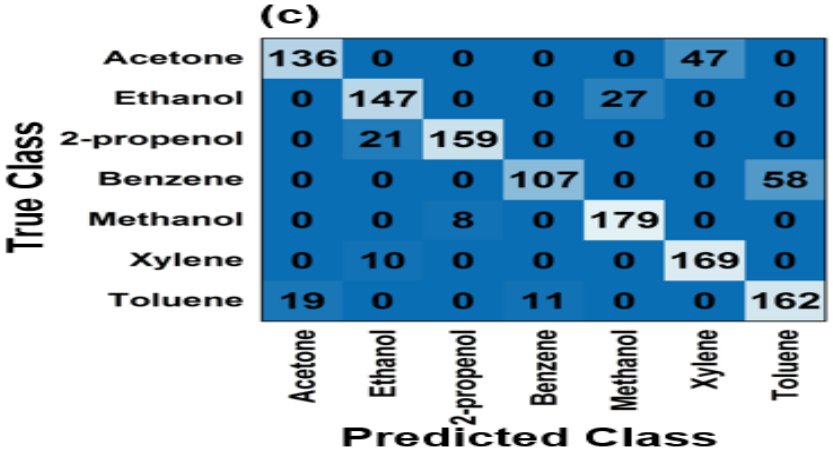
- Four different supervised algorithms were performed to determine the VOC
  - k-nearest neighbour (kNN)
  - Decision tree
  - Random forest
  - Multinomial logistic regression

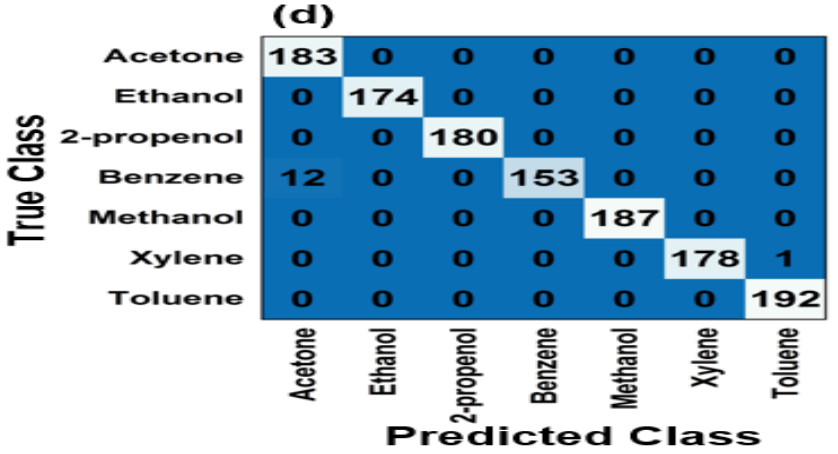
- An accuracy of 97.14%, 92.43%, 84.1%, 98.97% was obtained for kNN, decision tree, random forest, and multinomial logistic regression, respectively.

Confusion Matrix









(a) k-nearest neighbour (kNN)
(b) Decision tree
(c) Random forest
(d) Multinomial logistic regression

Conclusion

- Among PCA and LDA, LDA laid out the excellent separation between VOCs
- k-nearest neighbour and multinomial logistic regression performed outstandingly with an accuracy of 97.14% and 98.97%, respectively.
- Thus, high selectivity and accuracy authenticate that the system discriminates and differentiates multiple VOCs popularly exists in human breath.

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Thank You