## Development of Sensitive and Selective Solid State Gas Sensor System <u>Abstract</u>

The rapid rise in industrialization and standard of living, have led to many technological advances. Simultaneously, they have brought along several environmental problems and human safety concerns related to harmful gaseous/vapor emissions. In this regard, gas sensors find its wide range applicability in the area of environmental monitoring, indoor air quality, leakage/explosive detection, medical diagnosis, agricultural productions, food freshness, aerospace and many more. Thus, accurate, fast, sensitive, selective and real-time detection of target gas/volatile organic compound (VOCs) is a timely demand. Chemiresistive gas sensors (mainly metal-oxides) have been the most desirable candidate due to its many incredible properties, but they are deficient in the selectivity part.

This research work focuses on the development of gas sensor system featuring sensitive and selective detection of VOCs along with real-time monitoring outlook. Primarily, tin oxide (SnO<sub>2</sub>) with hollow-sphere morphology was employed as sensing material which demonstrated remarkable response with admirable sensitivity towards the tested VOCs, however the sensor showed huge cross-sensitivity which is intrinsic for any metal-oxide. The sensing material (SnO<sub>2</sub> hollow-sphere) was subsequently decorated with silver, gold, palladium and platinum to make an array of gas sensors, with the aim to improve the sensing performance in terms of lowered operating temperature and diverse sensing profile. The gas sensor array was exposed to different VOCs (acetone, benzene, ethanol, formaldehyde, methanol, 2-propanol and toluene) with varying concentrations. Interestingly, the combination of sensors presented diverse signatures from the collective response behavior to distinguish between the analytes selectively. Nevertheless, the approach was limited to obtain selective identification among the species for any particular fixed concentration. Next, a theoretical strategy was instigated where

the gas sensing kinetic parameters were extracted from the response transients based on adsorption/desorption of analytes over the sensing surface. The Eley-Rideal sensing mechanism was adopted for theoretical derivations, modelling and calculations. Eventually, distinct kinetic parameters that are associated with the tested VOCs were found which clearly exhibits discrimination among them. This proves to be an efficient way to identify different gas/VOC, as each analyte poses different kinetic properties such as reaction rate, activation energy. However, this methodology is purely theoretical requiring assumptions and therefore, not suitable for practical real-time detection. Finally, incorporation of machine learning (ML) tools was carried out to accurately identify the tested VOCs qualitatively and quantitatively. Different ML models were employed in supervised manner while exploiting various feature extraction techniques (steady state, signal transform, time series sequence) over the gas sensing dataset to check their credibility in terms of pattern recognition. A comparative analysis was carried out among different applied input features engaged with different ML models to examine their individual efficacy. The vigilant and efficient selection of features adequately allowed the ML models to achieve excellent classification and quantification which promote a step towards the realization of an automated and real-time detection. Particularly, a deep neural network model with time series response sequence as input information, delivered best performance with adaptive learning and fast prediction speed. Lastly, a smart and selective gas sensor system with assistance of machine learning was realized enabling wireless monitoring, internet connectivity and real-time user interface while empowering an essence of Internet of Things (IoT) paradigm. The present research work strengthens the next generation gas sensing technology for the progress of accurate, smart, selective, and miniaturized gas sensor devices for real-time applications.

**Keywords:** gas sensor, metal-oxide, chemiresistive, sensitivity, selectivity, tin oxide, volatile organic compound, gas sensing kinetics, machine learning, real-time, Internet-of-Things.