Novel Metal Oxide Semiconductor-Based Multifunctional Nanomaterials for Gas Sensing and Optical Applications

Submitted by: **Tanushri Das** Registration Number: **SOPHY1104721**
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Metal oxide semiconductor (MOS) nanomaterials-based chemiresistive gas sensors hold merits for its cost-effectiveness, simplicity of operation and stability. Selective detection of gases is crucial for environmental air-quality monitoring and diagnosing diseases by exhaled breath analysis. However, major drawback of binary MOS-based sensors is their low selectivity, slow response and recovery times, inability to detect gas in ppb concentration. This thesis delineates the exploration of novel MOS nanomaterials to overcome the drawbacks of the binary MOS gas sensors. Barium hexaferrite ($BaFe_{12}O_{19}$), a widely known magnetic material, has never been used as a gas sensor material before. The development of novel gas sensor is demonstrated based on $BaFe_{12}O_{19}$ nanoparticles, capable of detecting sub-ppm concentration of ammonia (NH_3) gas rapidly with high resolution while effect of interfering gases is minimum. The mechanism of NH_3 sensing of $BaFe_{12}O_{19}$ nanoparticles has been explained with the gas adsorption model. The excellent NH_3 sensing property of $BaFe_{12}O_{19}$ nanoparticles has proved its potential for practical application. With another exploration, substantial enhancement in response towards NH_3 by virtue of Zn-doping in $BaFe_{12}O_{19}$ has been observed. The enhanced sensing characteristics is attributed to the tuning of Fe^{2+}/Fe^{3+} ratio, oxygen vacancies and improved charge separation. Furthermore, simulated breath test validated the Zn-doped $BaFe_{12}O_{19}$ nanoparticles-based ammonia sensor's suitability for exhaled breath analysis. In another exploration, perovskite type bismuth ferrite ($BiFeO_3$), which is a multiferroic material, has been studied for its gas sensing activity. Pure and Sn-doped $BiFeO_3$ nanoparticles exhibited ppb-level formaldehyde (HCHO) detection. The enhancement of HCHO sensing property is a combined effect of charge compensation mechanism due to valency mismatch, improved charge-separation and enhanced oxygen defects generated in the system. Excellent HCHO sensing activity of Sn-doped $BiFeO_3$ nanoparticles indicates its potential towards the monitoring of indoor air quality. In the next study, the formation of n-n-type heterostructure between $MoO_3/BiFeO_3$ for its hydrogen sulfide (H_2S) gas sensing capability has been demonstrated. Utilizing photoelectrochemical measurement, the electron transfer mechanism from conduction band (CB) of $BiFeO_3$ to the CB of MoO_3 has been revealed. This study provides a route for designing bandgap-engineered α-$MoO_3/BiFeO_3$-heteostructure with enriched oxygen defects to address the need for environmental air-quality monitoring. Finally, for optical study, $NaTb(MoO_4)_2$ nanoparticles has been explored. In addition, $NaTb(MoO_4)_2$ exhibited formaldehyde (HCHO) sensing activity with outstanding response characteristics. The formation of band structure has been studied by employing density functional theory (DFT). Excellent green photoluminescence property of disordered $NaTb(MO_4)_2$ structure revealed its potential for commercial use in light emitting devices. Moreover, the gas response characteristics has established $NaTb(MO_4)_2$ nanoparticles as a novel HCHO sensing material suitable for real-time air quality monitoring. This study provides new insights into the fabrication and engineering of nanomaterials that exhibit multifunctionality driven by structural disorder. In totality, a combined study of different types of MOS nanomaterials and their heterostructures for gas sensing and optical properties have been delineated. Improved gas sensing property has been achieved for these materials in terms of sensitivity, response time and low concentration gas detection which overcomes the demerits of binary MOS-based gas sensors. Some of the materials have exhibited both photoluminescence and gas sensing property. Both of these properties are controlled by surface electronic states, charge transfer mechanism and structural disorder in the system. All of these investigated materials can positively contribute to efficient gas sensing and optical applications.

Signature of the supervisors with seal: **Signature of the candidate:**

Ghosh 19/09/24
Dr. Chandan Kumar Ghosh
Asst. Prof., School of Materials Science & Nanotechnology, Jadavpur University

Dr. Chandan Kumar Ghosh
Assistant Professor
School of Materials Science
& Nanotechnology,
Jadavpur University
Kolkata - 700 032

Mrinal Pal 19/9/24
Dr. Mrinal Pal
Chief Scientist & Head,
FMDD, CSIR-CGCRI

Dr. Mrinal Pal
Chief Scientist & Head
Functional Materials and Devices Division
CSIR-Central Glass & Ceramic Research Institute
Kolkata- 700 032

Tanushri Das. 19/09/2024
Tanushri Das
Jadavpur University