Poster Presentation

International Winter School 2021 on Frontiers in Materials Science

Design and Development of Metal-Organic Framework based Materials for Gas Sensing Applications

Presented By: Ms. Marilyn D Mello

CSIR-Senior Research Fellow

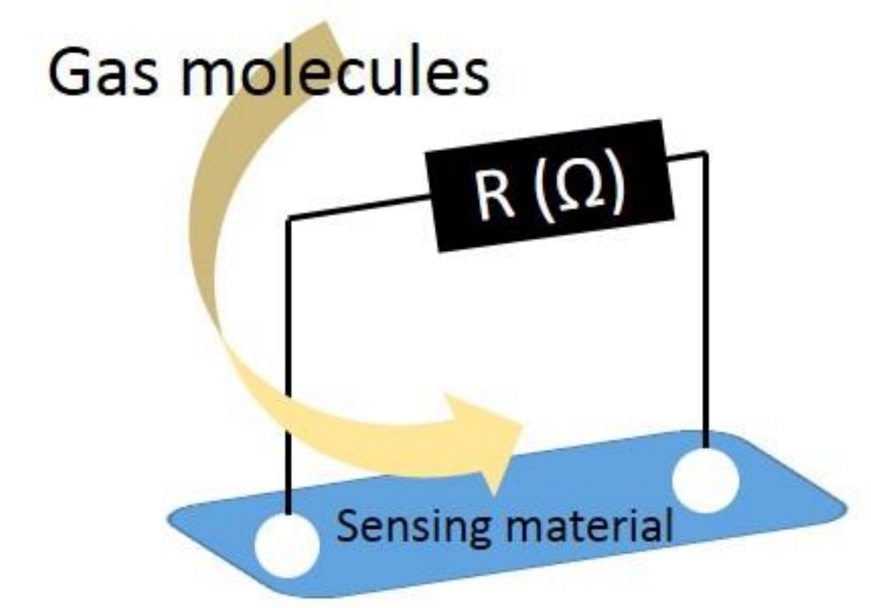
Guide: Dr. Suresh Babu Kalidindi

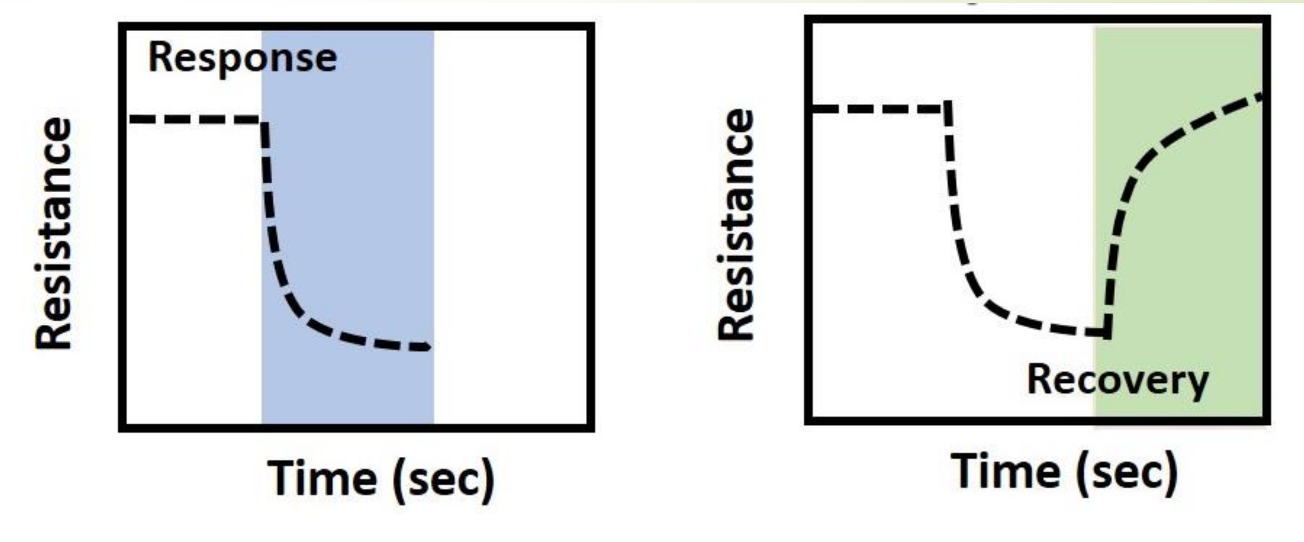
Co Guide: Dr. Ganapati V Shanbhag

Poornaprajna Institute Of Scientific Research, Bangalore, India

Chemiresistive Gas Sensing

- The performance of a chemiresistive sensor largely depends on the analyte interaction with the surface of the sensing element.
- Measurement of changes in the electrical resistance induced in the sensor materials.
- Resistivity based sensors are quite promising because of simple instrumentation, rapid analysis and low cost.

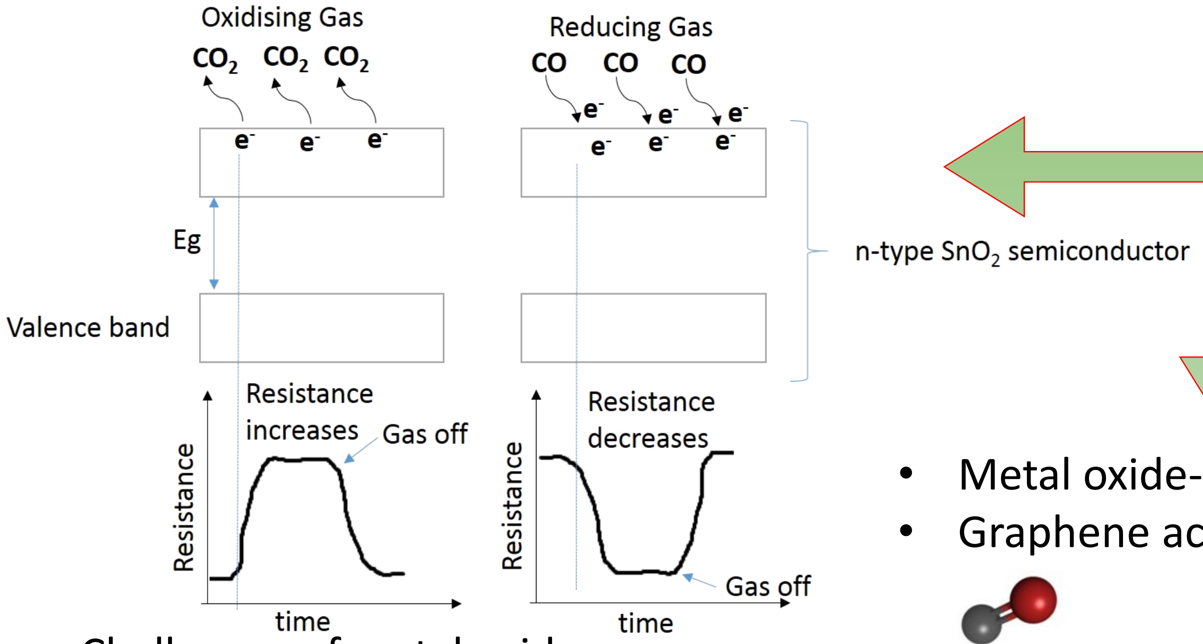




Our approach for chemiresistive gas sensing

Metal Oxides

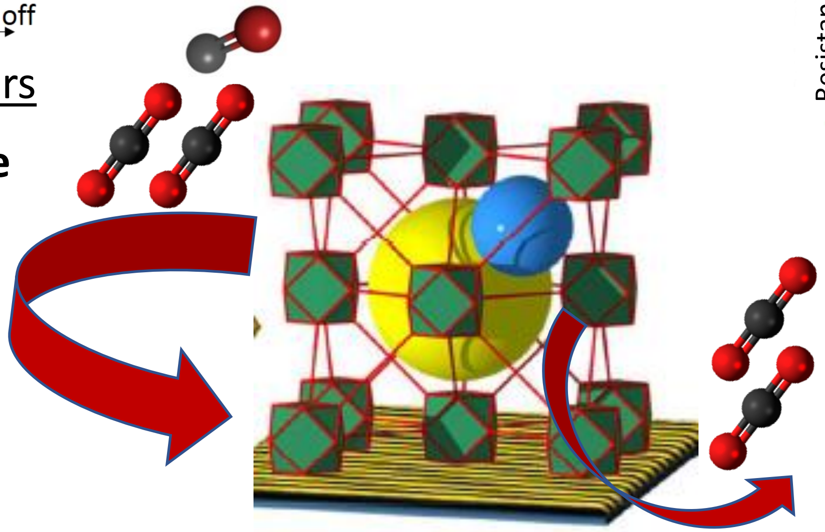
- **Low cost, easy production, low electrical resistance and compact size.**



Challenges of metal oxide gas sensors

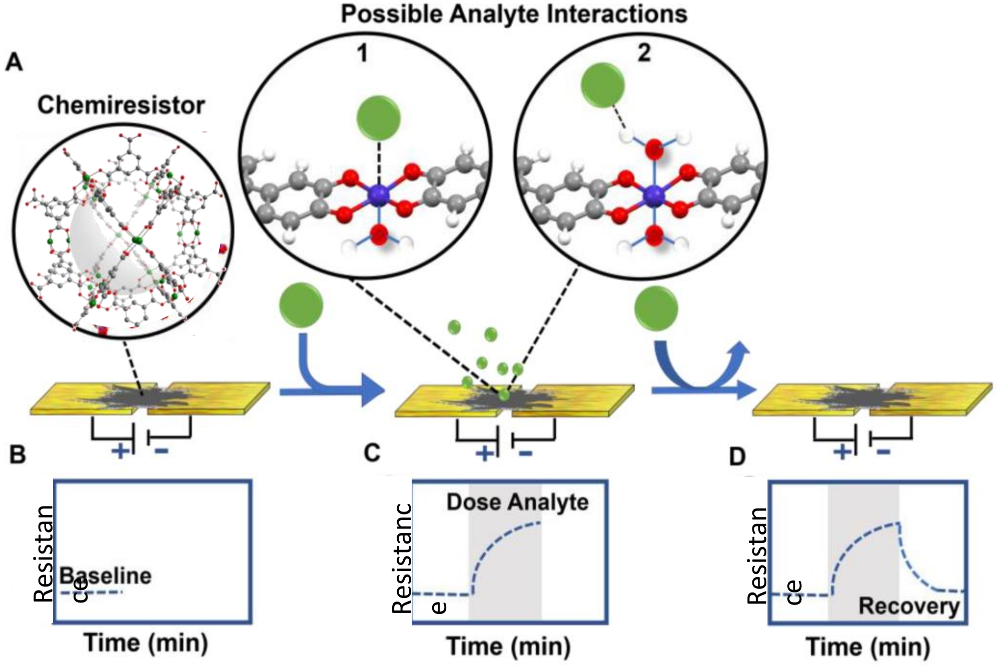
- **Sensors require a high temperature (200–400 °C) to achieve optimum measurements.**
- **Limited on low surface areas**
- **Lack of selectivity to a particular analyte**

- Metal oxide-MOF Hybrid
- Graphene acid-MOF Hybrid



Metal-Organic Frameworks(MOFs)

MOFs are porous crystalline materials constructed by joining metal- containing units [secondary- building units (SBU)] with organic linkers.

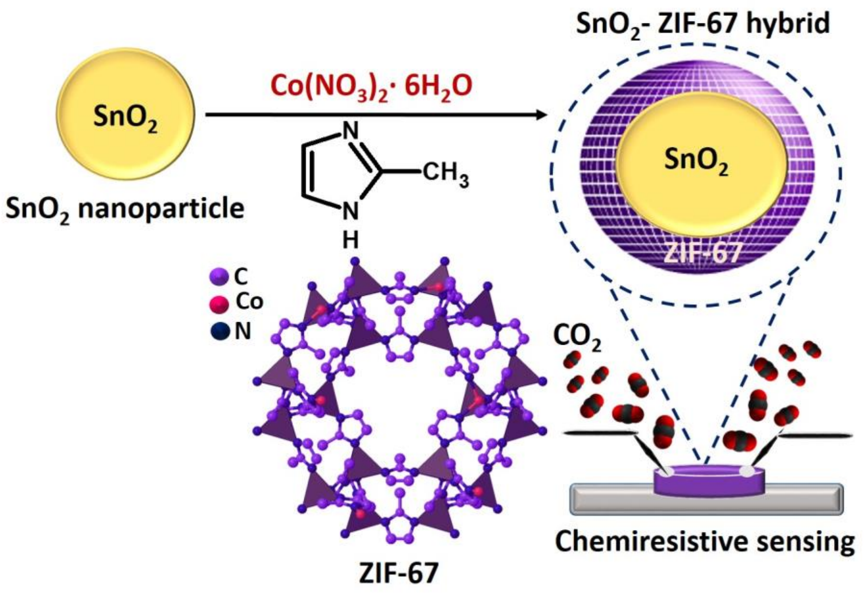


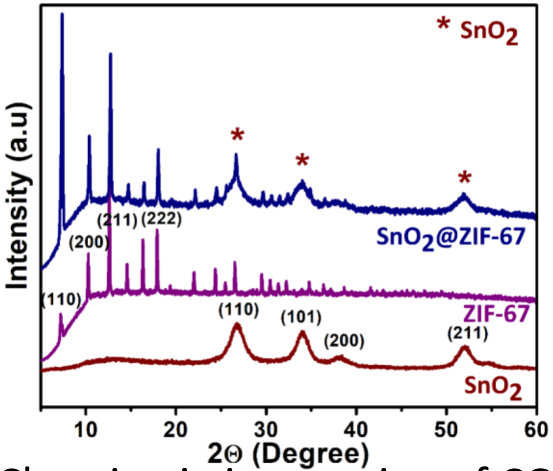
Interesting Properties:

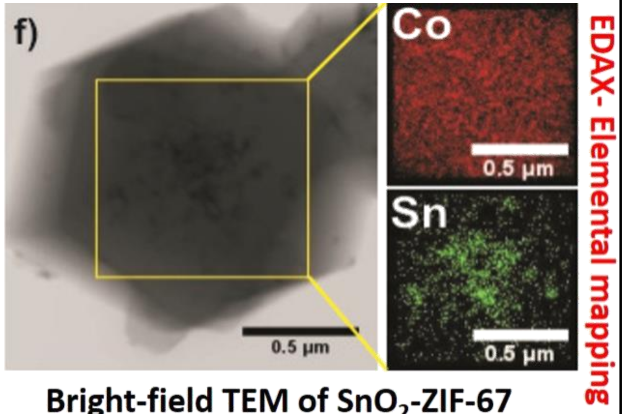
- **Rational design**
- **Large pore volume**
- **High surface area**
- **Flexible nature**
- **High chemical and thermal stability**

Our Materials design Strategy

Metal oxide-MOF Hybrid



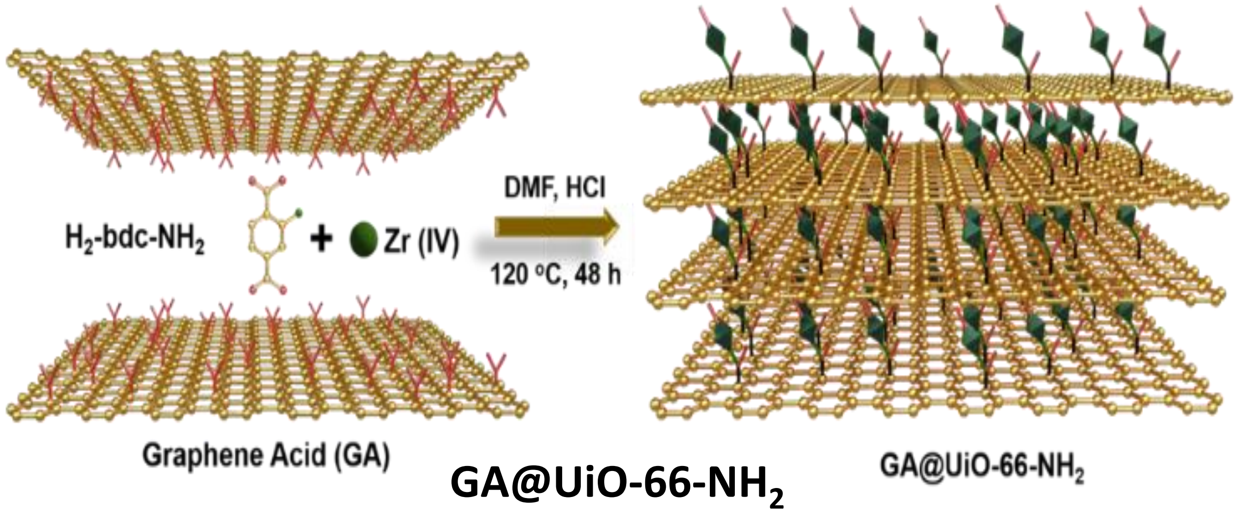




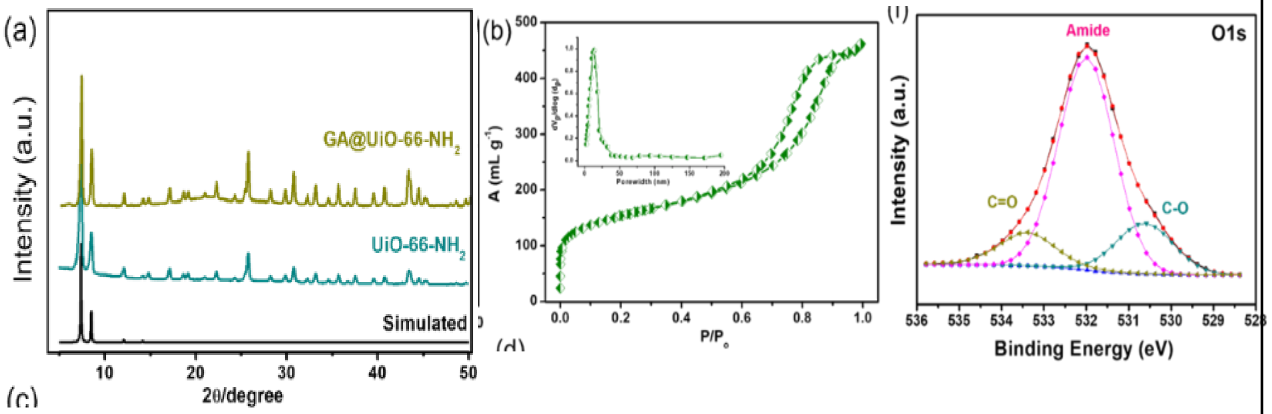
Bright-field TEM of SnO$_2$-ZIF-67

Chemiresistive sensing of CO_2 gas from 500 ppm to 50 % concentration.

Graphene acid-MOF Hybrid



GA@UiO-66-NH$_2$

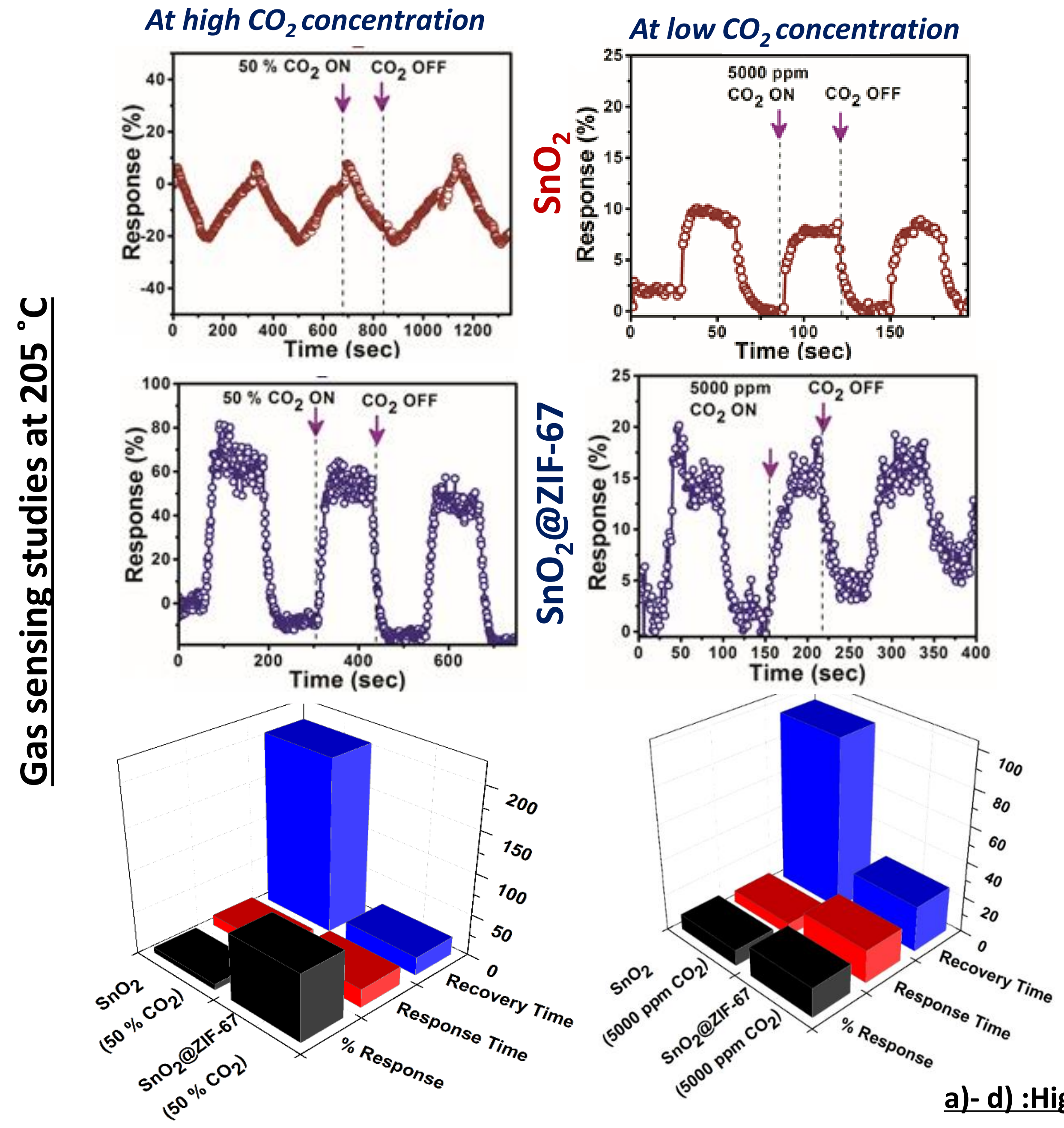


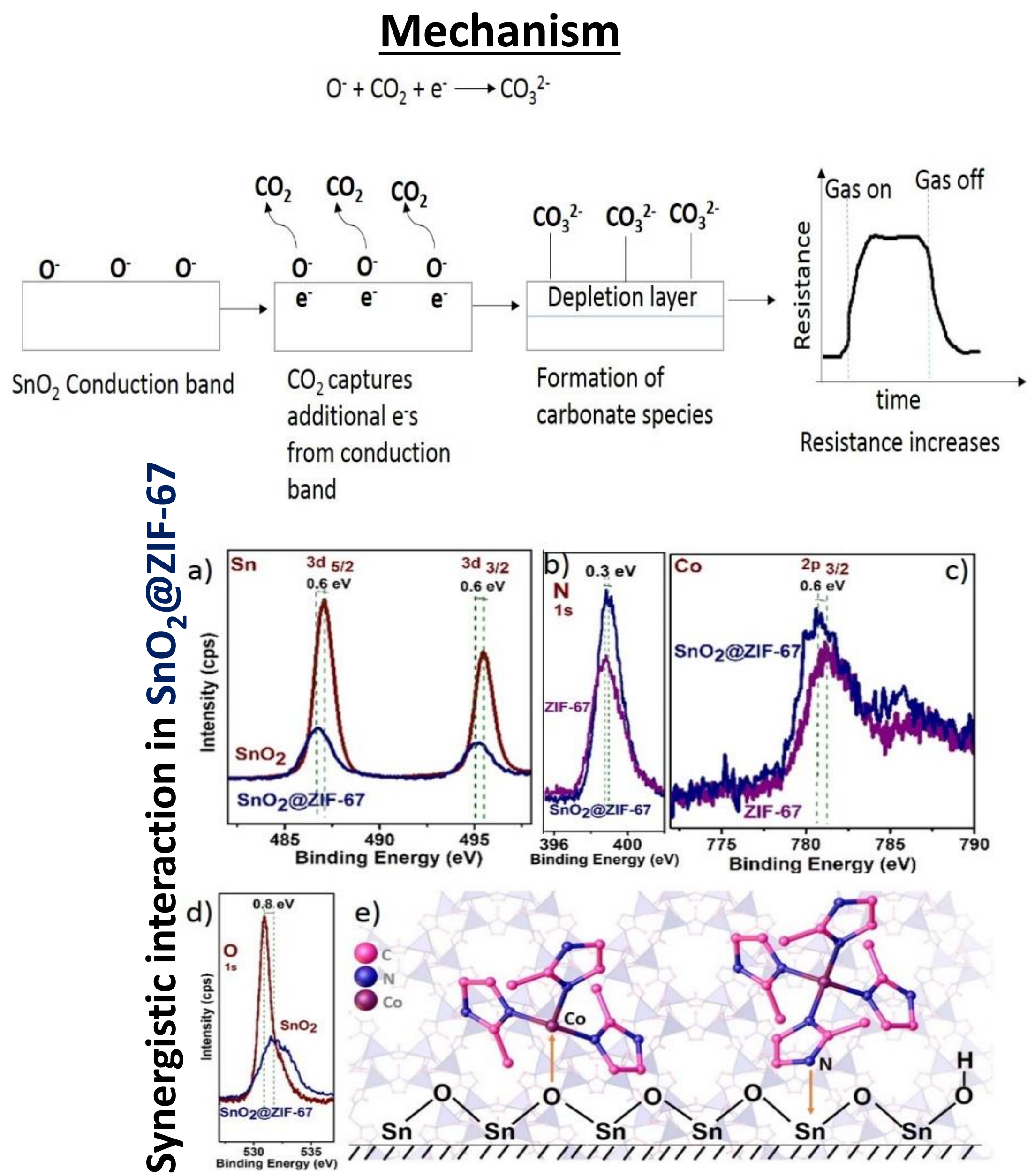
Chemiresistive sensing of CO_2 attributed to the better interaction of CO_2 at the amide/amine functional groups and the readily accessible hierarchical pores .

Chem. Eur. J., 2018, **24**, 9220–9223

J. Mater. Chem. A, 2021,**9**, 17434-17441

Assembly of ZIF- 67 Metal-Organic Framework over Tin Oxide Nanoparticles for Synergetic Chemiresistive CO_2 Gas Sensing

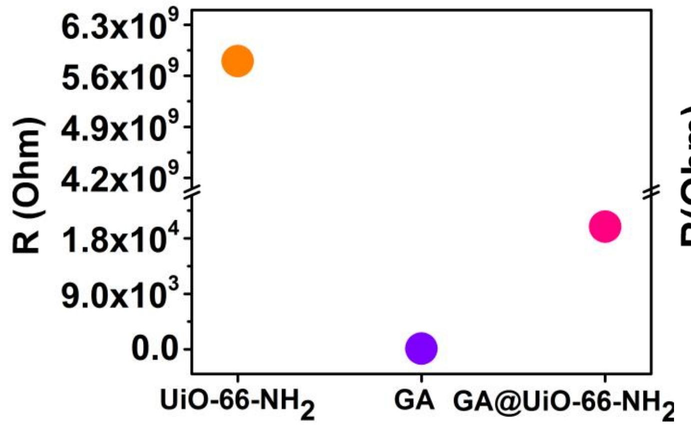


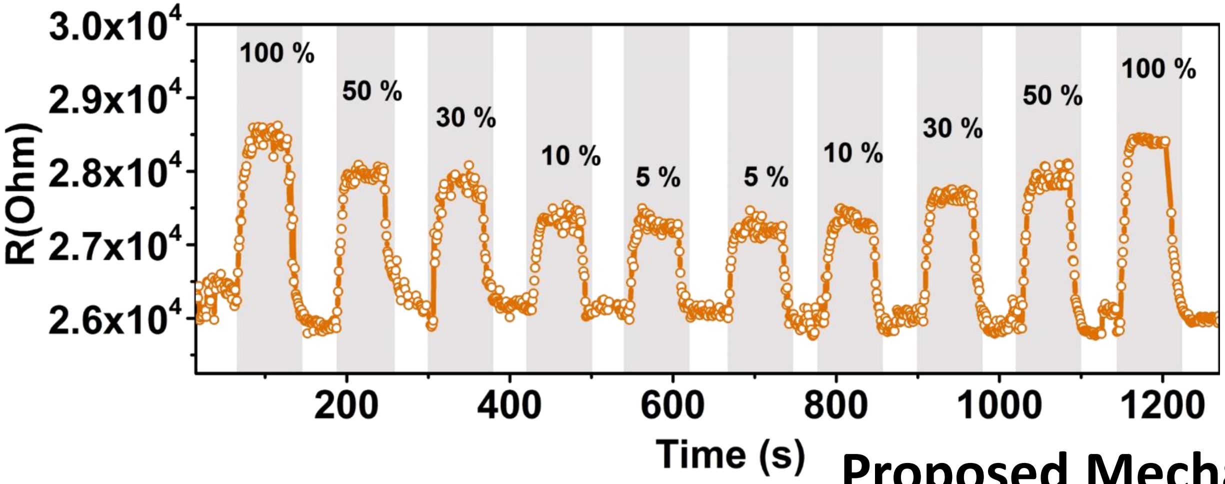


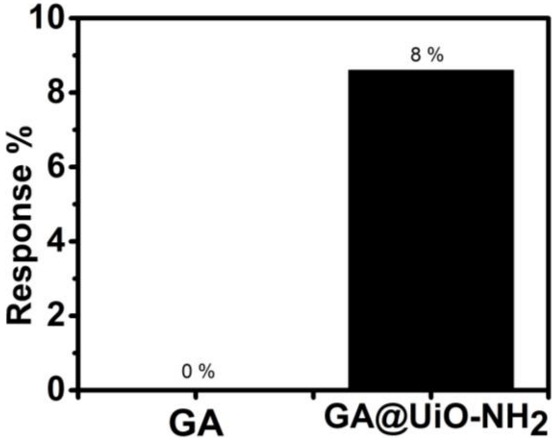
a)- d) :High resolution X-ray photoelectron spectra of SnO_2 and SnO_2@ZIF-67 materials

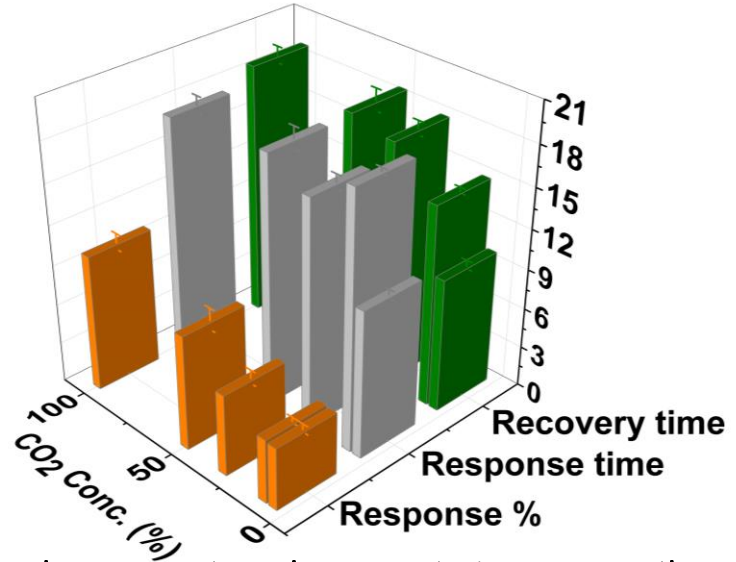
Multifunctional Covalently Linked Graphene-MOF Hybrid as an Effective Chemiresistive Gas Sensor

Gas sensing studies with GA@UiO-66-NH_2 (Zr) hybrid at 200 ˚C

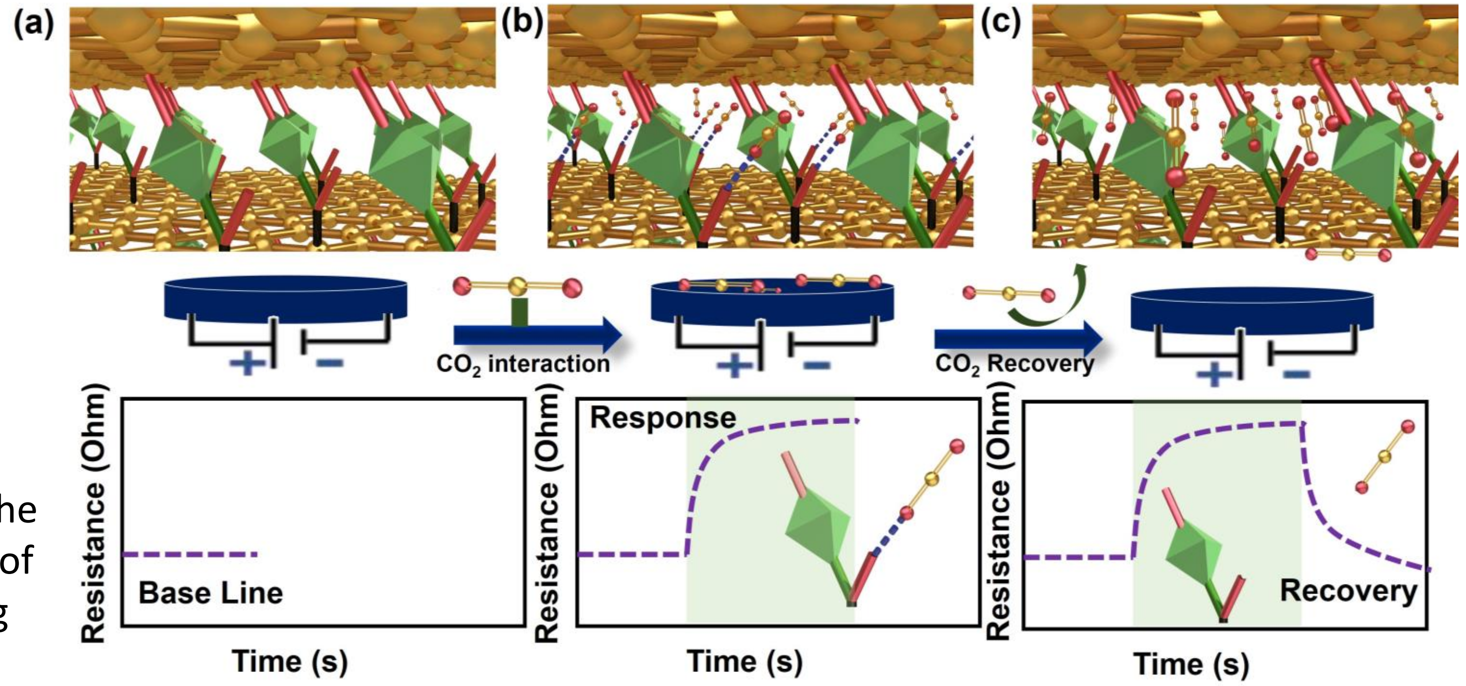








Proposed Mechanism



The novel CO_2 sensing characteristics are attributed to the synergistic effect between GA and UiO-66-NH_2 in terms of good conductivity, hierarchical porous nature facilitating gas diffusion and amide-based interaction sites.

Conclusion

- We have designed, synthesized and tested hybrids of Metal Oxide-MOF (SnO_2@ZIF-67) core-shell and Graphene acid-MOF (GA@UiO-66-NH_2) for chemiresistive gas sensing application.
- We targeted sensing of a important gas- CO_2 in the present study as they have vital significance in safety and industrial processes.
- Unlike SnO_2, which showed an ambiguous low response, the SnO_2@ZIF-67 exhibited a stable and strong response owing to synergistic effects (such as electronic structure changes) arising from the hybrid nanostructure in case of the first study.
- And in the second study, GA@UiO-66-NH_2 showed a response for CO_2 while pristine GA exhibits negligible response under the same conditions.
- Overall, the nanostructures of SnO_2@ZIF-67 and GA@UiO-66-NH_2 opens new horizons in the development of MOF based hybrids displaying high selectivity with rapid response and recovery times for the detection of greenhouse gases like CO_2.

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