2D Materials for Gas Sensing

S. Guo, A. Rani, and M.E. Zaghloul

Department of Electrical and Computer Engineering

The George Washington University, Washington DC 20052

Outline

- Background
- Structures of 2D Material for Gas Sensing
- TMDS Material
- Examples of 2D material for gas sensing and Results
- Conclusion and Future Work
- Acknowledgement

Background

- Recently 2D materials have been used for gas sensing because of the atomic-thin layered structure, large surface-to-volume ratio, and large adsorbing capacity of gas molecules and strong surface activities.
- Recently layered inorganic material analogues of graphene, such as Transition Metal Dichalcogenides (TMDs) were developed .
- These material include MoS_2 , WS_2 , $MoSe_2$, WSe_2 , ReS_2 , and $ReSe_2$, as well as layered metal oxides (MoO_3 and SnO_2) .
- Unlike graphene, TMDs monolayers have the potential to exist in more than one possible crystal structure. This implies :
    - Semiconducting (2H) phase
    - Semi-metal (1T’) phase
    - Tunable Band gap, high sensitivity for varieties of chemicals.
    - Thickness dependent Physical and Chemical properties .

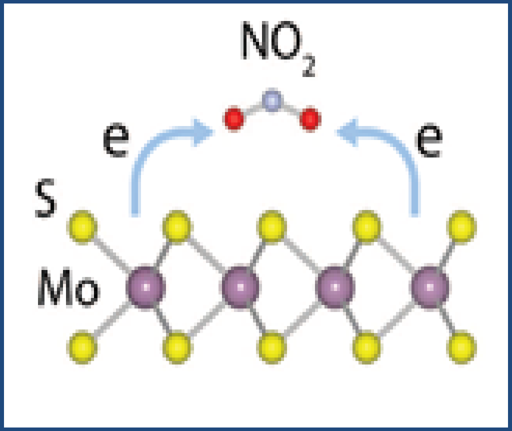
Gas Sensing Mechanism

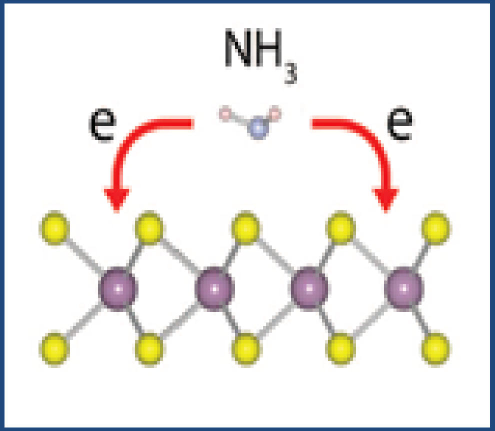
- The Gas sensing mechanism is based on transfer of charges, in which the sensing material acts as absorber or donors of charges.

- The charge transfer between the gas molecules and the sensing material will cause changes in the sensing material properties.

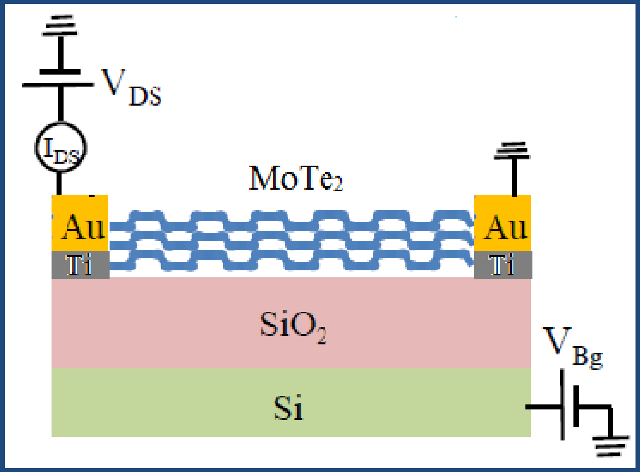
Semiconductor gas sensing mechanism

Classification	Oxidising Gases	Reducing Gases
N-type	R increase	R decrease
P-type	R decrease	R increase





Gas Sensing Device (FET) structure



Structure of the FET Device

- The gas sensor works by bridging the two electrodes (source and drain) with sensing materials and passing current through them.
- Gas detection can be realized by monitoring the current change upon exposure to the target gas environment under a constant voltage.
- For conductance type gas sensor, both high sensitivity and fast recovery rate are desirable.

Various Types of 2D Gas Sensing devices

- There are several structures of 2D material Gas sensing devices, examples of such devices are:
  - Chemiresistor Sensors
  - Field Effect Transistors FETs
  - Schottky diodes
  - Conductometric sensors
  - Surface Acoustic Wave (SAW) sensors

Performance Parameters

- The performance parameters for gas sensing are characterized by:
  - Sensor Response Time
  - Selectivity
  - Sensitivity
  - Stability
  - Recovery Time

Performance Parameters Factors

- The Gas sensor Performance is influenced by several parameters:
  - The sensing material type and dimension
  - Humidity
  - Temperature
  - Gas flow rate

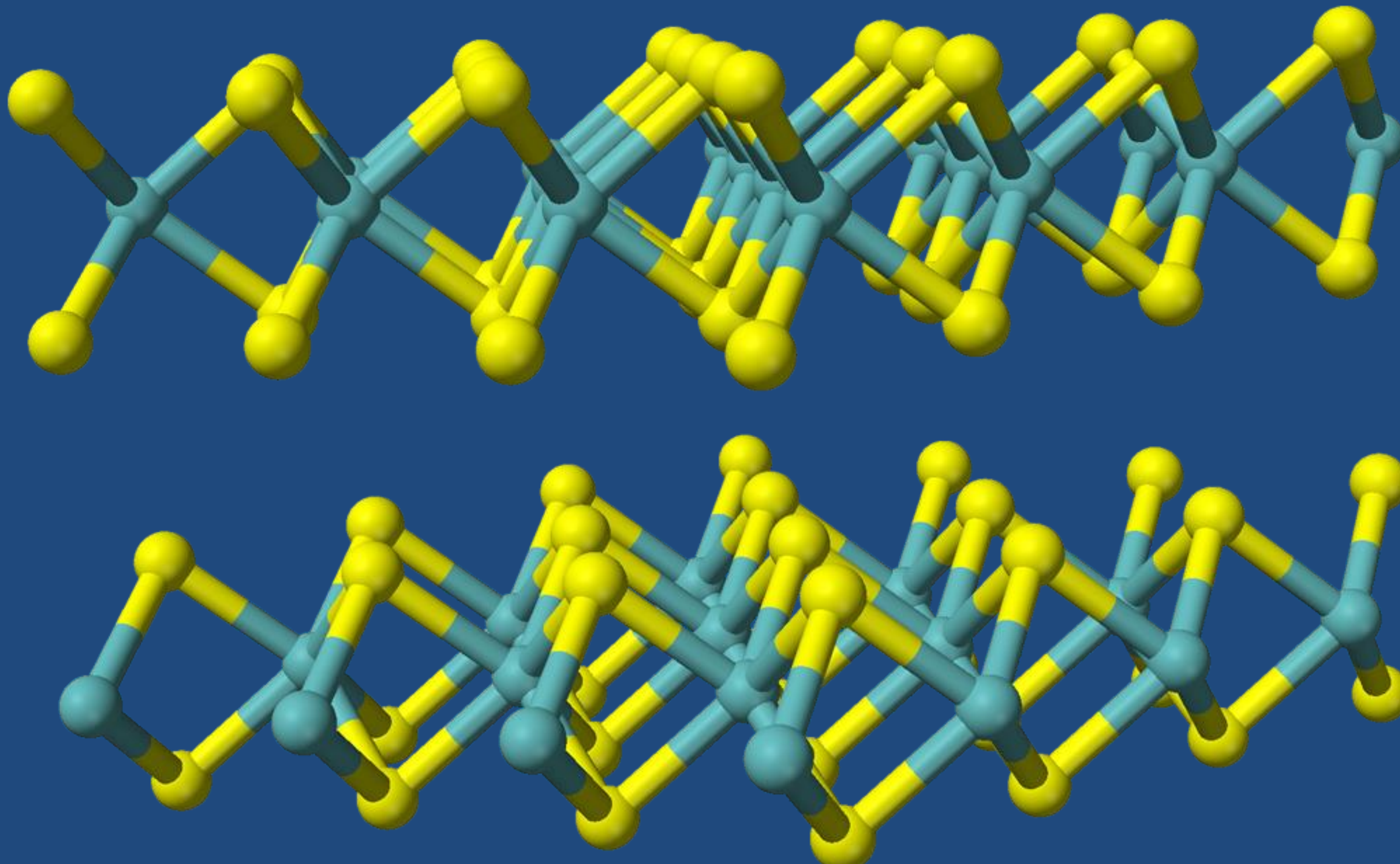
There are several approaches to improve the performances of the sensor such as using programming temperature , the use of UV light into the sensor, and the use Nano Particles as catalyst to improve absorption and thus improve selectivity.

Our Group Research on Gas Sensing

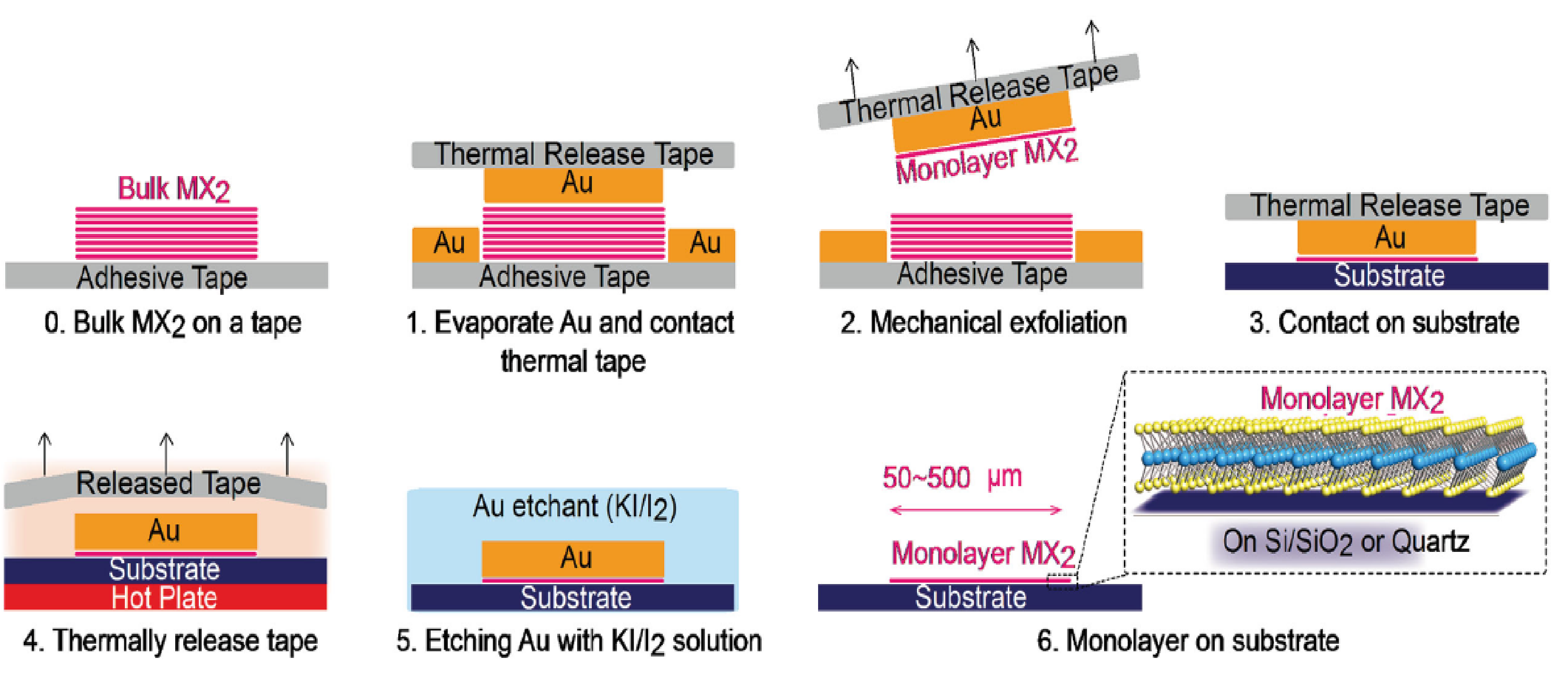
- We are studying gas sensing properties for two TMDs materials:
  - $MoSe_2$
  - $MoTe_2$

Gas sensors using $MoSe_2$

- Molybdenum diselenide ($MOSe_2$)
- An inorganic compound, its structure is similar to MoS_2
- Single Crystal layers of $MoSe_2$ and flakes are exfoliated from bulk Crystal
- Electron mobility of 2D $MoSe_2$ is higher than MoS_2
- It has direct band gap

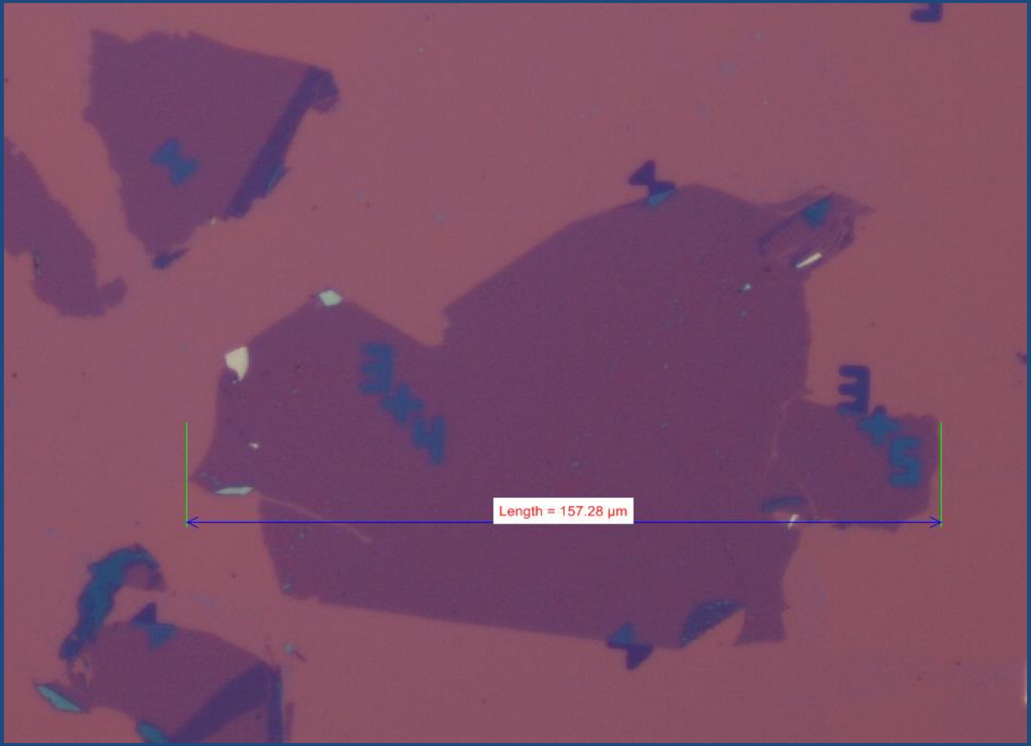


Transfer material
Gold Assisted Exfoliated



Ref : Sujay B. Desai et al.; Gold-Mediated Exfoliation of Ultralarge Optoelectronically-Perfect Monolayers; Adv. Mater. 2016, 28, 4053–4058

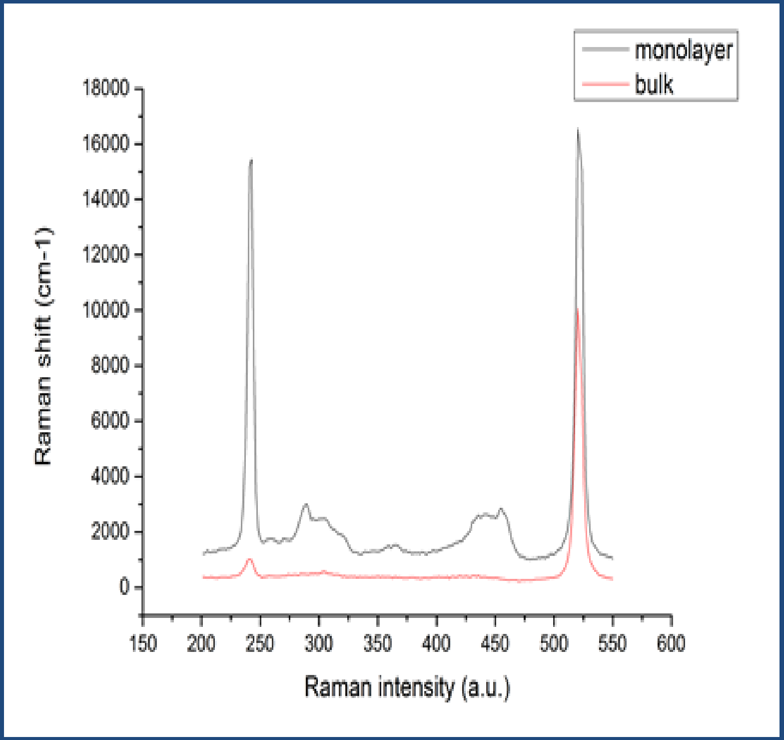
Flakes Transferred



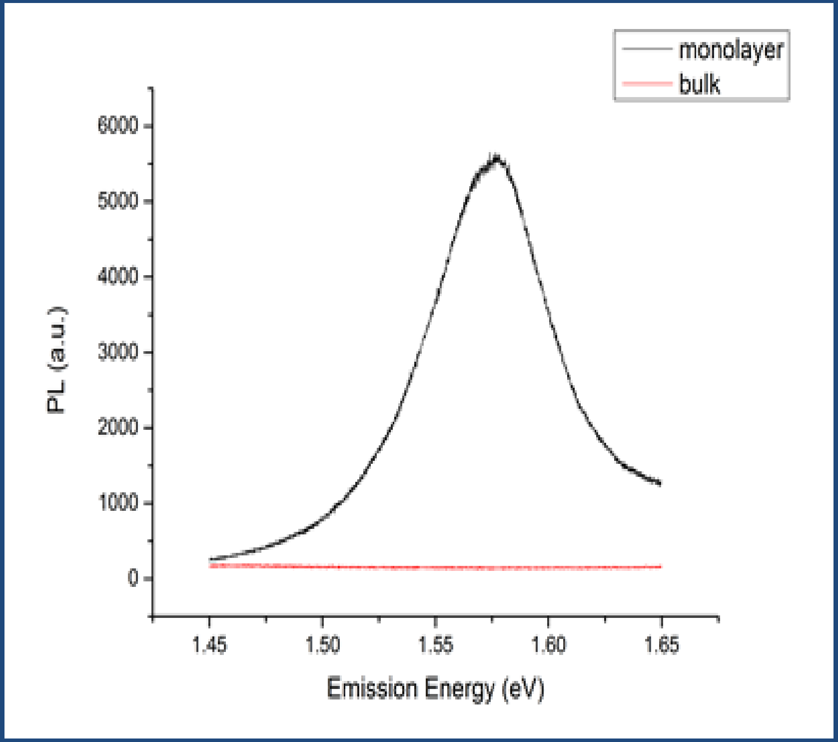
Optical image of transferred flake

MoSe2 Characterization using Raman and PL

Raman Spectra



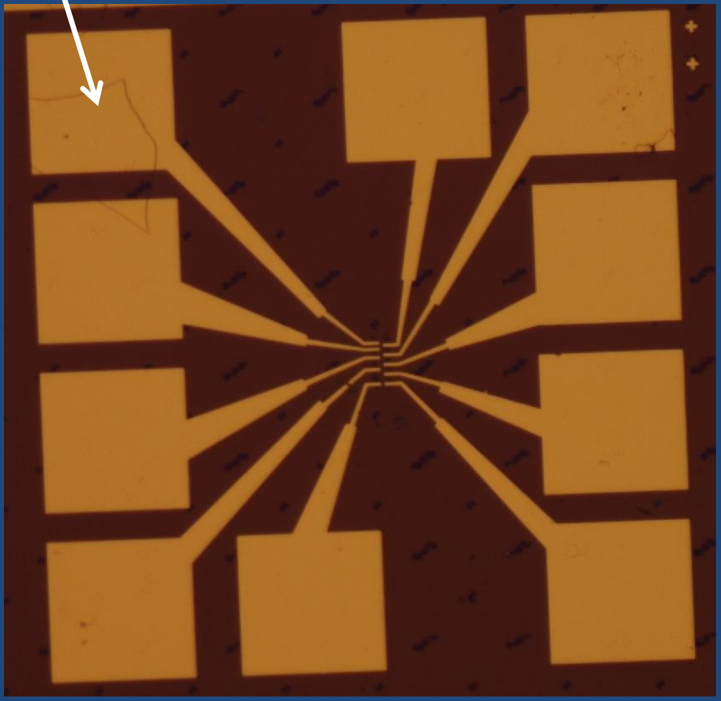
PL



Mask and Optical image of the device

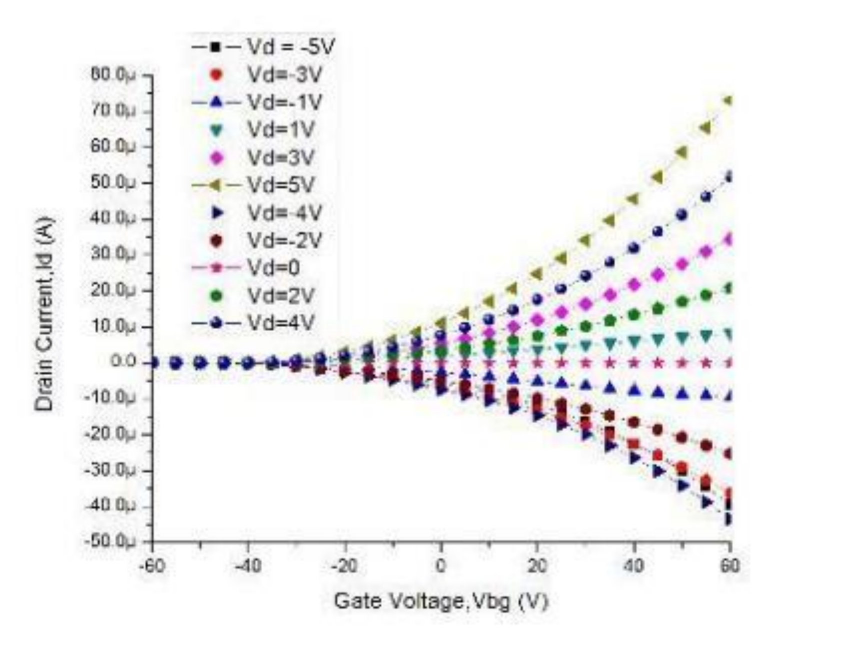
Contact Pad

Etched channel

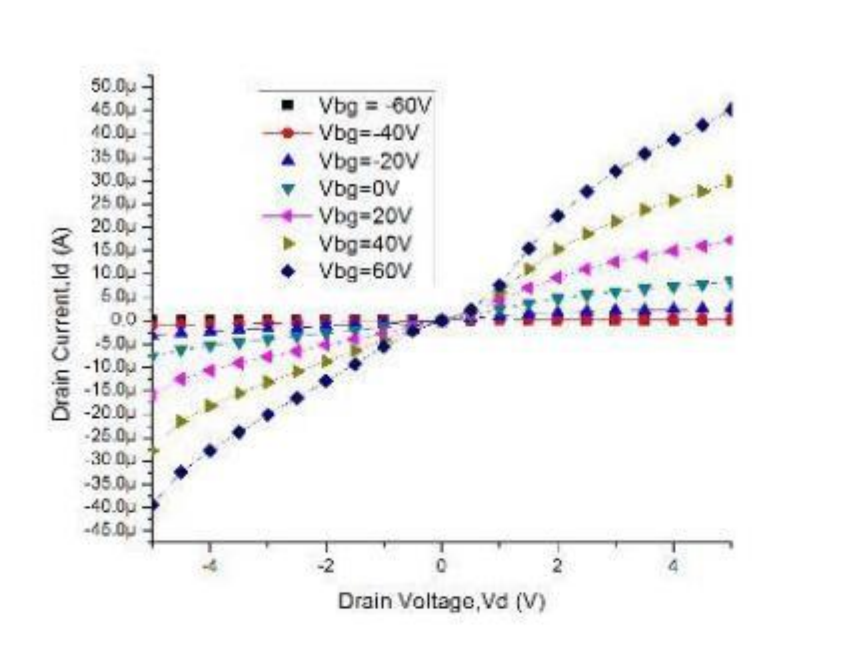


FET characteristics (n-type)

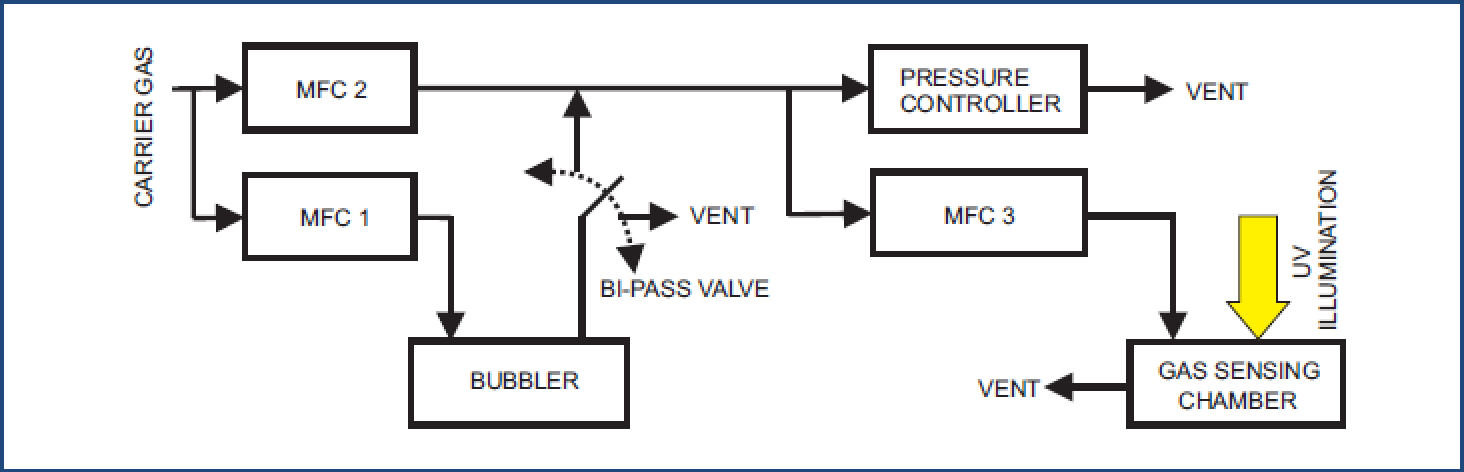
Transfer Characteristic



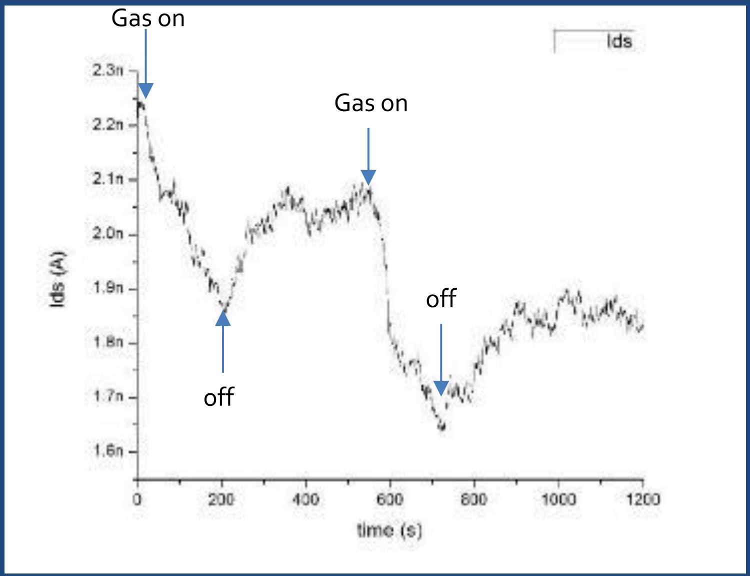
Output Characteristic

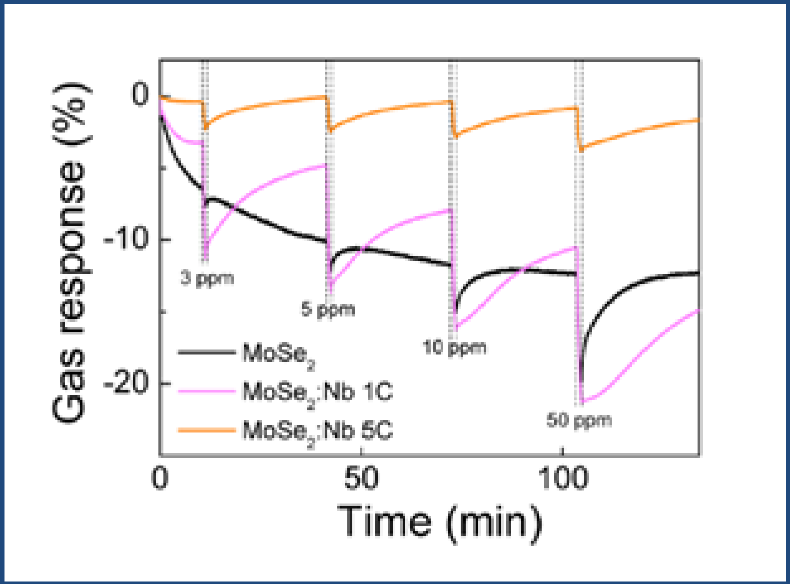


Gas sensing set up Structure



Gas response (20ppm NO_2)





Sun Young Choi et al.; Effect of Nb Doping on Chemical Sensing Performance of Two-Dimensional Layered MoSe2; ACS Appl. Mater. Interfaces 2017, 9, 3817–3823

In comparison, $MoSe_2$ always have large recovery time which we need to find a way to improve. Our device can reach 20% response for 20ppm NO2 and shows great sensitivity.

Challenges with the measured Data

- Large recovery time 400s
- How to improve the sensitivity in the range of 100ppb - 10ppm
- How to improve the selectivity

Work we are doing to improve the results

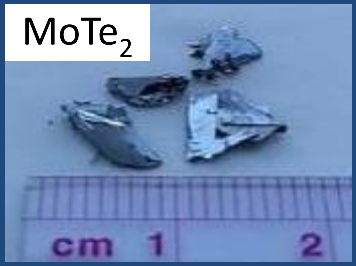
1. Heat assist to help recovery

2. FET structure/UV assist to help improve sensitivity

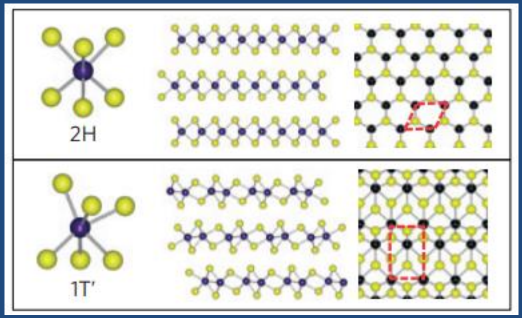
3. Metal nanoparticles decoration to help improve selectivity

$MoTe_2$

- Molybdenum ditelluride ($MoTe_2$) is an especially attractive 2D material because it exists in two stable polymorphs.

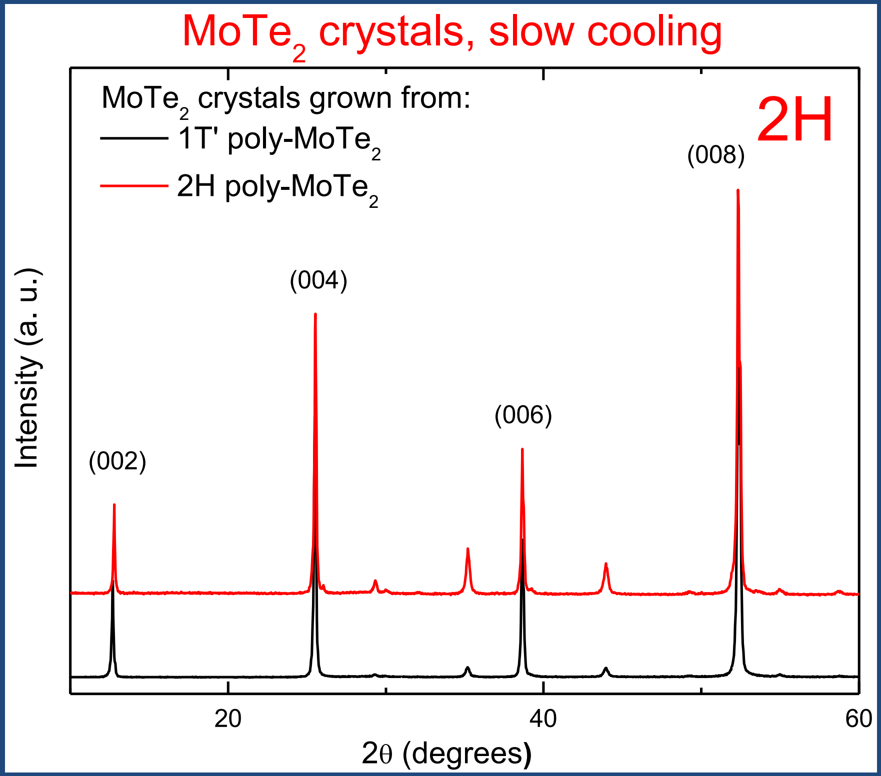


1. Semiconducting hexagonal (2H) and
2. Semi-metallic monoclinic (1T')



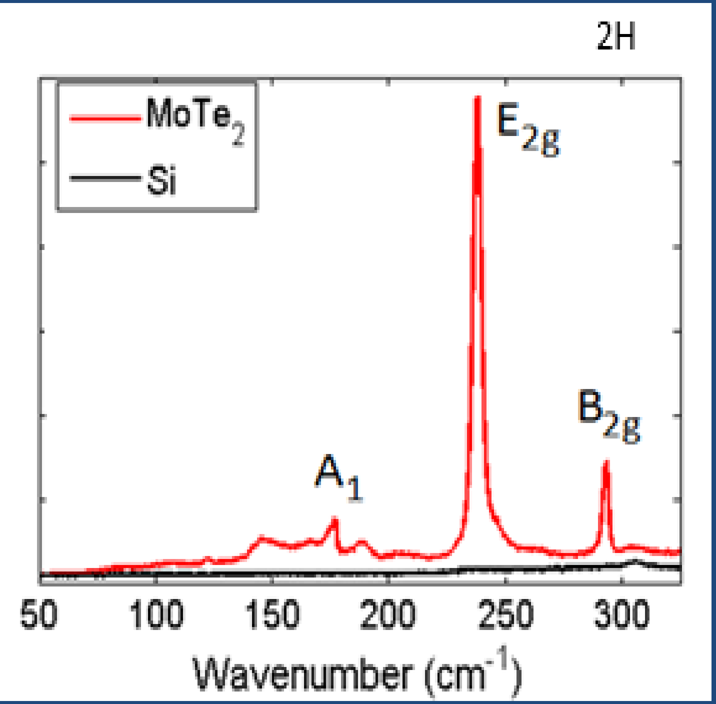
Two phases can be reversibly transformed by altering $MoTe_2$ crystal growth conditions or by a post-growth thermal treatment.

$MoTe_2$ 2-D Material
Material Characterization of 2H-$MoTe_2$



- Cooling rate defines a crystal structure of $MoTe_2$ single crystals, regardless of the initial crystal phase of the poly-$MoTe_2$.
- X-Ray diffraction patterns were obtained using milled $MoTe_2$ powders and platelets.

Material Characterization of 2H-$MoTe_2$

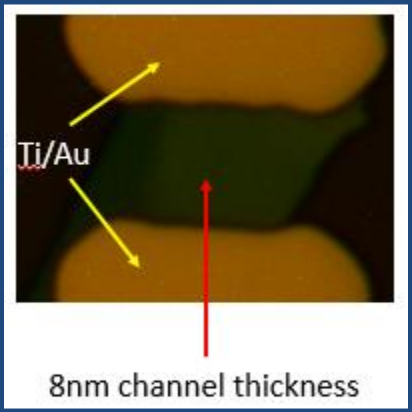


- Raman spectra were acquired from the 2H- $MoTe_2$ flakes exfoliated onto SiO_2/Si substrates. The spectra for the 2H flakes, exhibit an out-of-plane A_g mode around 170 cm^{-1}, an in-plane E_{2g} mode around 235 cm^{-1} and an out-of-plane B_{2g} mode at 289 cm^{-1}.

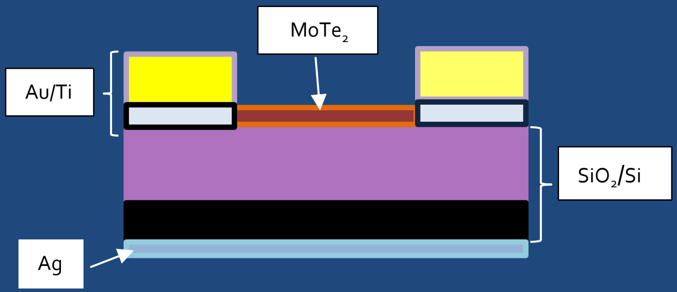
- All lines are in excellent agreement with Raman studies reported in the literature [14, 15], which confirms the phase and quality of the flakes.

Electrical Characterization

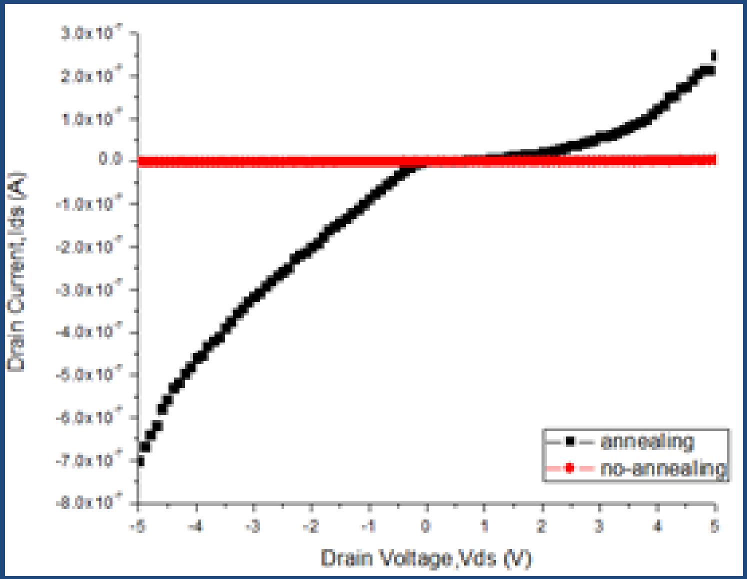
Optical Image



Schematic



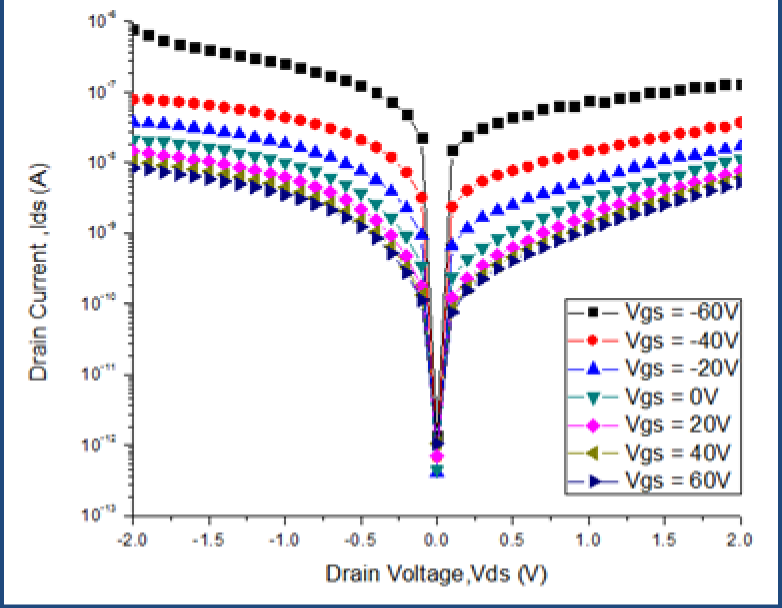
Current Voltage graph



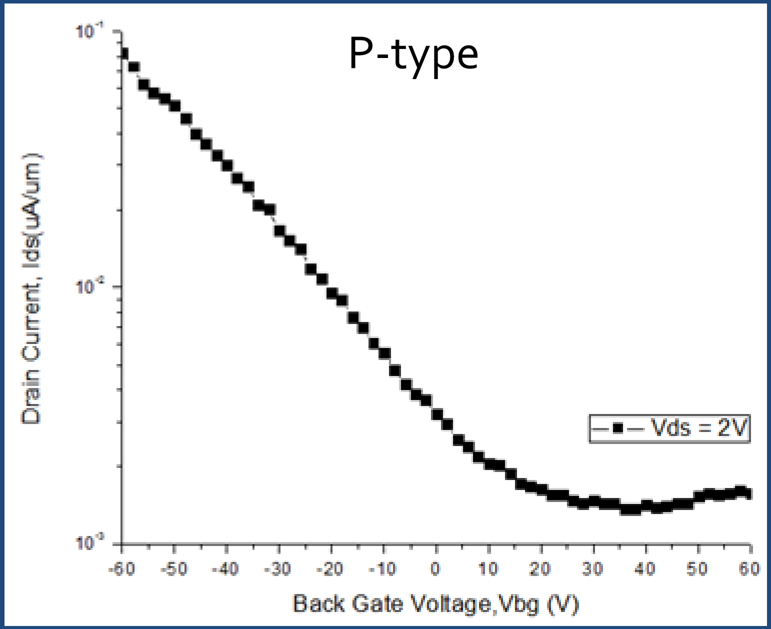
Annealing was done at 350 °C

Electrical Characterization

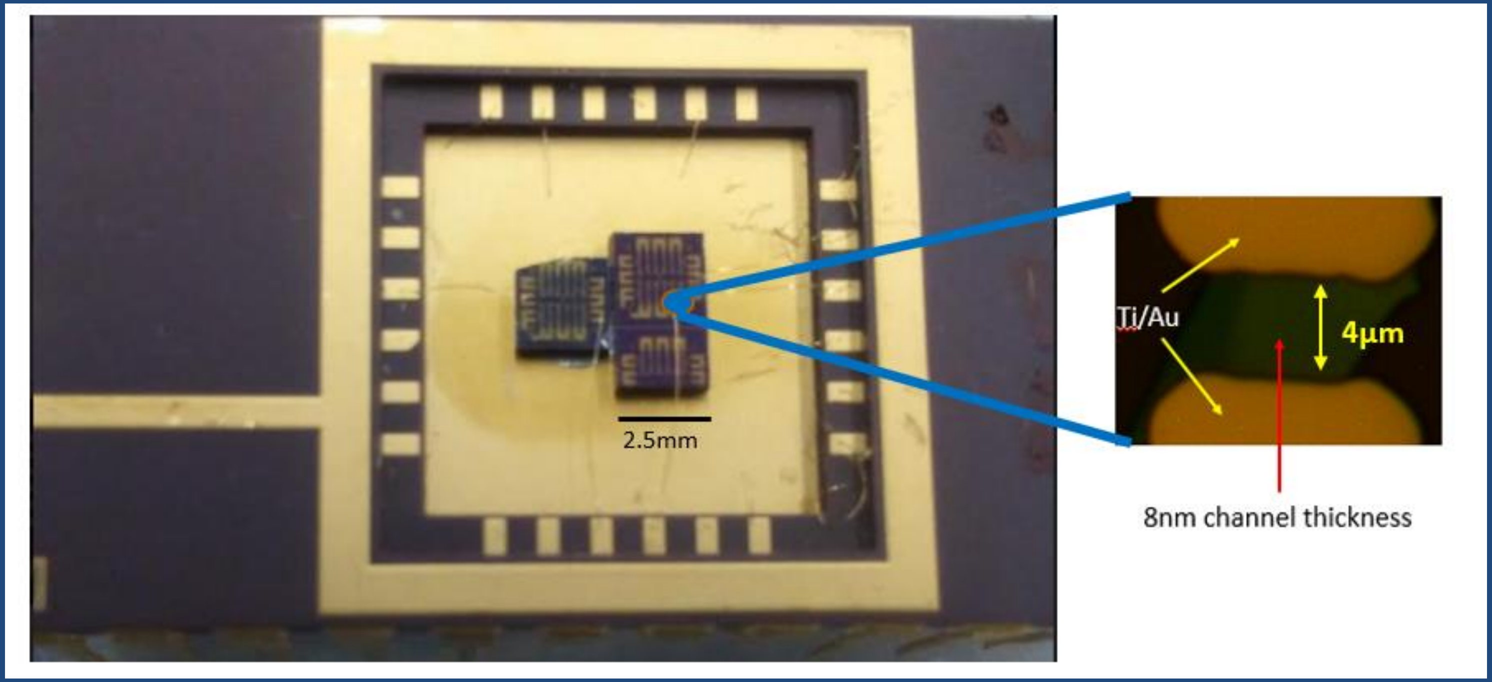
Output Characteristic



Transfer Characteristic



Packaging of $MoTe_2$ For gas sensor



Three different thickness $MoTe_2$ FET are packaged on above chip-career for gas-sensing measurement.

Approaches to improve the Gas-sensing performance

1. Incorporation of UV light into gas sensors.
2. High sensitivity can be achieved by good Schottky barrier modulation of 2D material and metal electrode junction.
3. Surface functionalization of the 2D channel between source and drain electrodes.

   Example : Pt nanoparticles on MoS_2 thin films.
4. Decoration of 2D material with metal oxides.

   Example : MoS_2/SnO_2 channel between source and drain electrode.
5. Annealing the 2D sensing material at proper temperature.

Summary

- It is an important to develop Very sensitive and Very selective gas sensing device for many applications such as health, food, agriculture, …
- Two dimensional (2D) material is showing great potential in gas sensing with high sensitivity due to their high surface-to-volume ratio and promising semiconductor properties.
- Our Goal is to develop portable wearable gas sensing device

Acknowledgement
NIST Collaborators

- Dr. Albert Davydov : Supervisor
- Dr. Sergiy Kylyuk : Growth of material
- Dr. Ryan Beams : Raman Spectroscopy
- Dr. R. Debnath : Electrical Characterization
- Irian Kalish : X-Ray Diffraction