



## Miniaturized Sensors for Explosives Detection in Air

**Jan Larsen**

**DTU Informatics**



**A Strategic Network**

**Total Budget: 29.200.000 DKK**

**Funded by the Danish Agency for Science and Technology  
Program Commission on Nanoscience, Biotechnology and IT (NABIIT):  
14.990.200 DKK**

**Project Coordinator: Professor Anja Boisen, DTU Nanotech**

slides based on Mogens Havsteen Jakobsen's presentation at the NDRF workshop on Molecular and Odour Detection 05.03.2008

# Xsense

## Project Partners



**DTU Informatics**

Department of Informatics and Mathematical Modeling



**DTU Nanotech**

Department of Micro- and Nanotechnology



UNIVERSITY OF SOUTHERN DENMARK

**SERSTECH**

TOMORROW'S TECHNOLOGY AVAILABLE TODAY



**Unisensor**

**DTU Informatics**

Department of Informatics and Mathematical Modeling

Technical University  
of Denmark





## Motivation

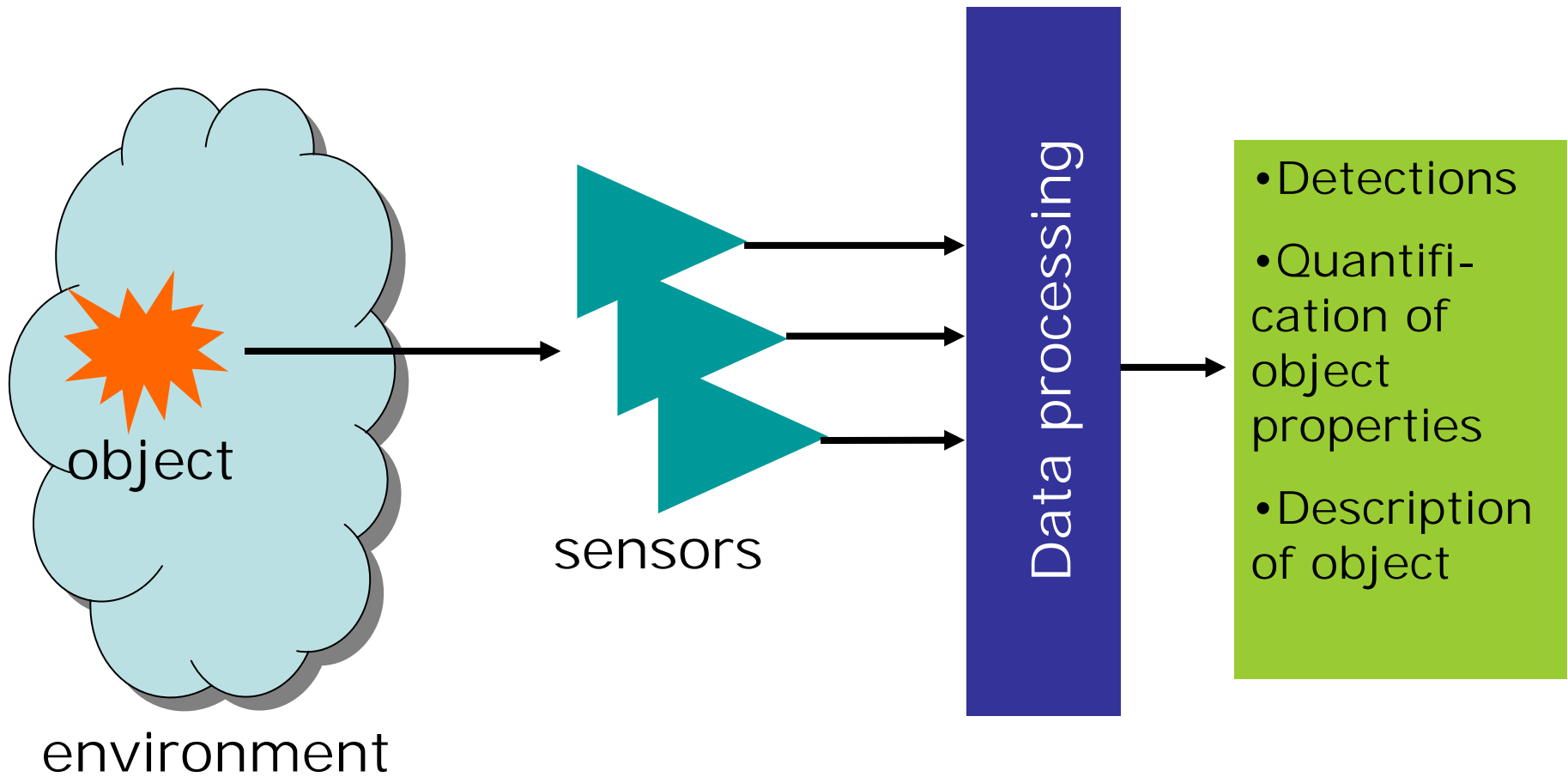
**In the future development of sensor based explosives detectors we find that the key challenges to address are:**

**reliability, selectivity, stability and cost.**

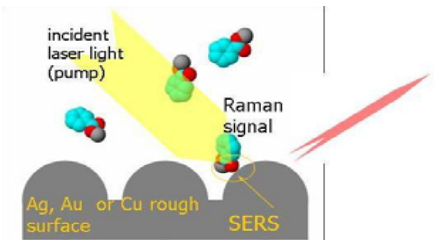
**Our hypothesis is that only by combining several independent and sensitive measuring principles can the reliability be improved.**

**We will do this by creating a strategic research network with significant pre-existing know-how and strong competences in:**

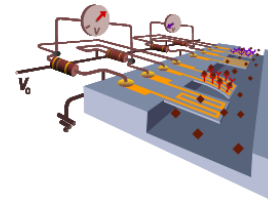
**miniaturized sensors, synthetic chemistry,  
surface functionalization, data processing and validation.**



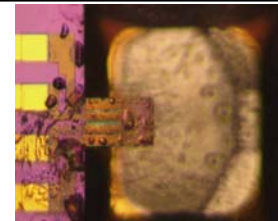
**Surface Enhanced Raman Spectroscopy (SERS)**



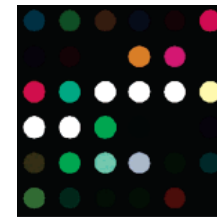
**Cantilever Sensors**



**Micro Calorimetric Sensors**



**Colorimetric Sensor Arrays**





## Other Major Activities

- **Sample Preparation / Pre-Concentration**
- **Data Processing and Sensor Networks**

### **Not considered**

- Environment models
- Modeling of explosive transportation and degradation

# Surface enhanced Raman Spectroscopy on Chip

Jorg Hubner, Thomas Anhøj, Sarah Pedersen, Dan A.Zauner, Anders M. Jørgensen, Gabriella Blagoi, Ivan Talian and Ole Hansen

*DTU Nanotech - Department of Micro and Nanotechnology, Technical University of Denmark*

# Principles of Raman Spectroscopy

Raman effect:

- Weak interaction between molecule vibrations and light.
- By exposing a molecule or molecules to specific light the molecules starts vibrate and emits a spectrum of light.

ingerprint of a molecule.

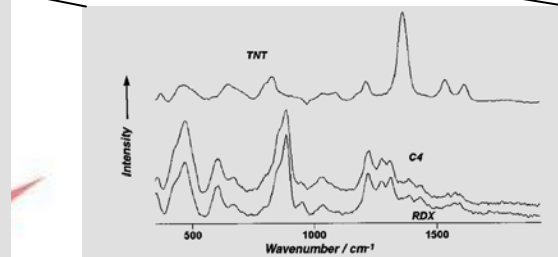
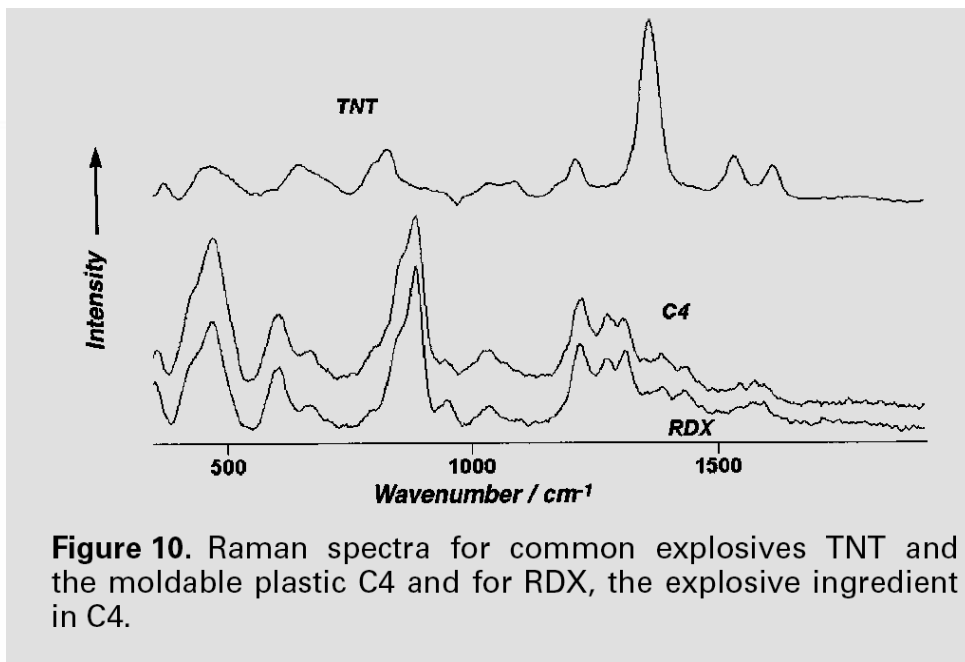


Figure 10. Raman spectra for common explosives TNT and the moldable plastic C4 and for RDX, the explosive ingredient in C4.

Clarke et al., J. Raman Spectr. 30, 827-832 (1999)

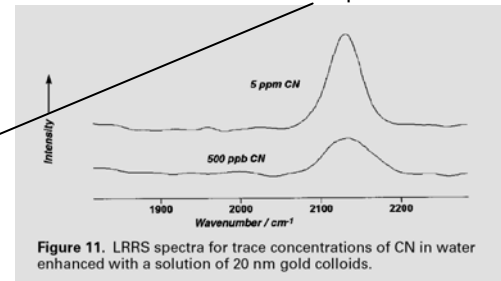


Figure 11. LRRS spectra for trace concentrations of CN in water enhanced with a solution of 20 nm gold colloids.



## Principles of SERS

### Surface Enhanced Raman Spectroscopy:

- To enhance emitted light from a molecule it can be attached to a surface.
- Enhancement of the interaction between molecules and light up to a factor 1.000.000.000 (or more in special cases) can be achieved utilizing a nano structured metal surface.

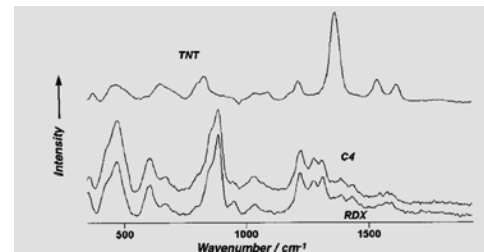
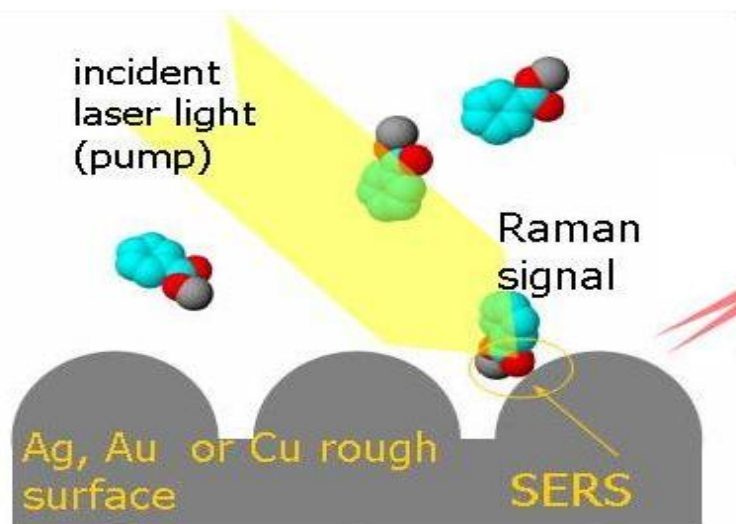


Figure 10. Raman spectra for common explosives TNT and the moldable plastic C4 and for RDX, the explosive ingredient in C4.

Clarke et al., J. Raman Spectr. 30, 827-832 (1999)

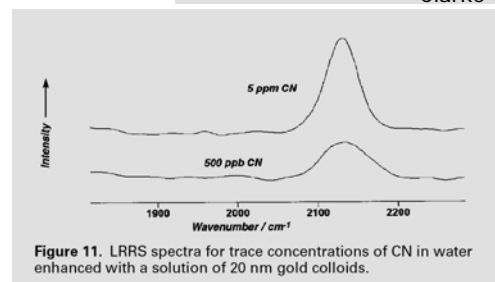
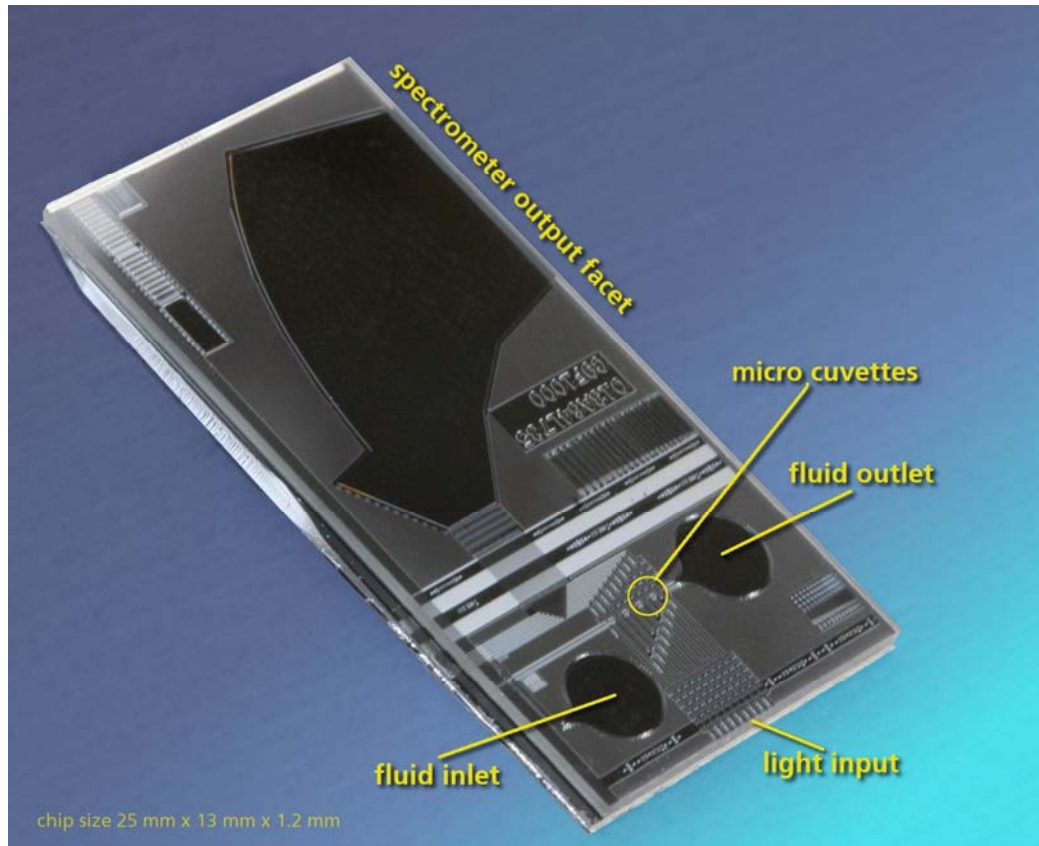


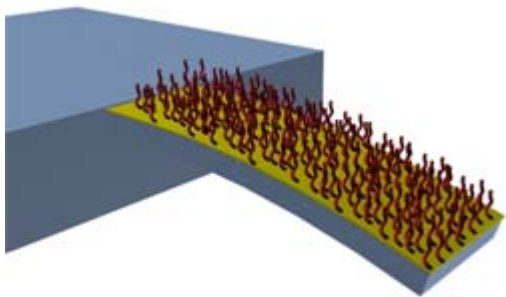
Figure 11. LRRS spectra for trace concentrations of CN in water enhanced with a solution of 20 nm gold colloids.

## The Spectrometer Chip with Optic and Fluidic Circuitry

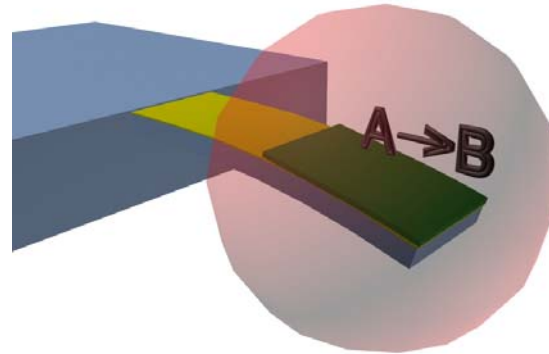


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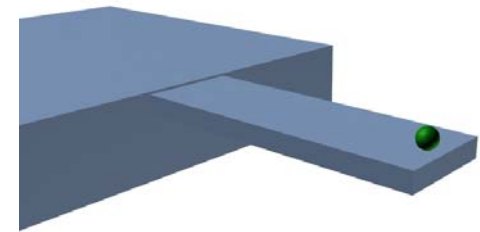
## Cantilever Sensors



**Change of surface stress**



**Change of temperature**



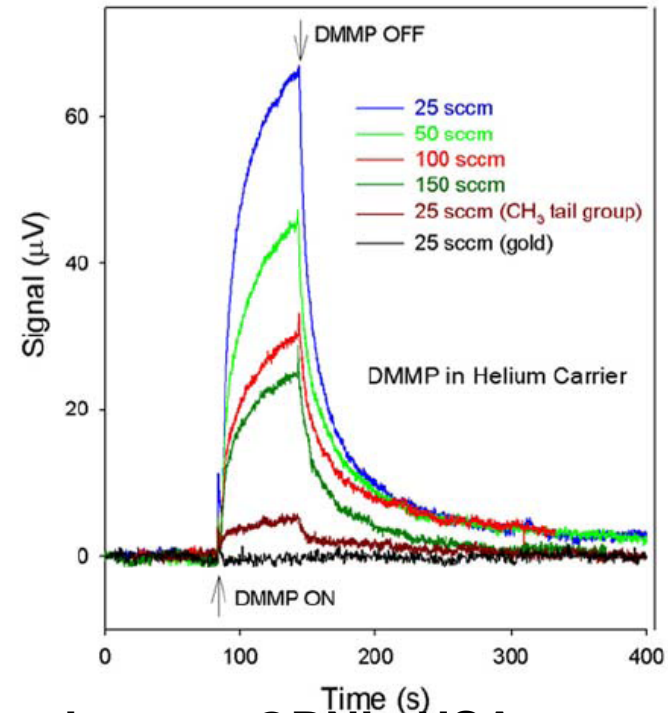
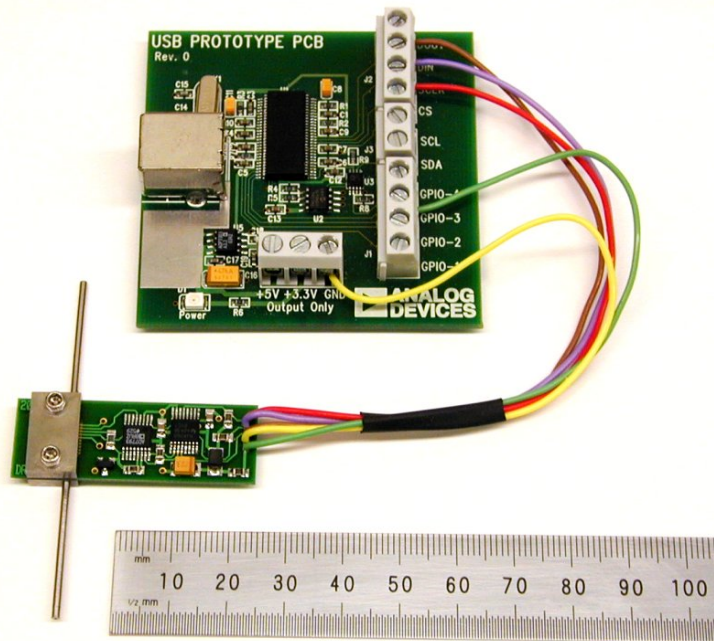
**Change of mass**

**Gene/Protein  
detection**

**Antigen/antibody  
recognition**

**Gas detection**

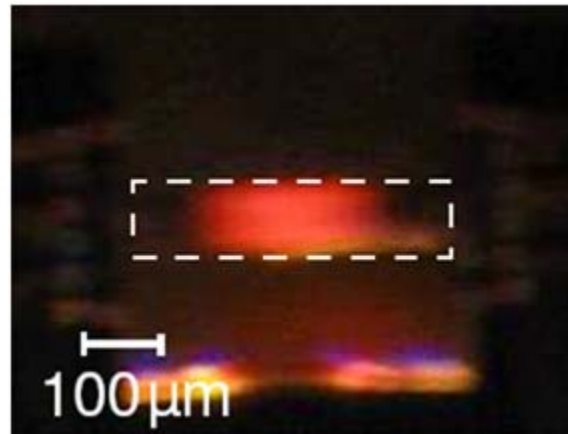
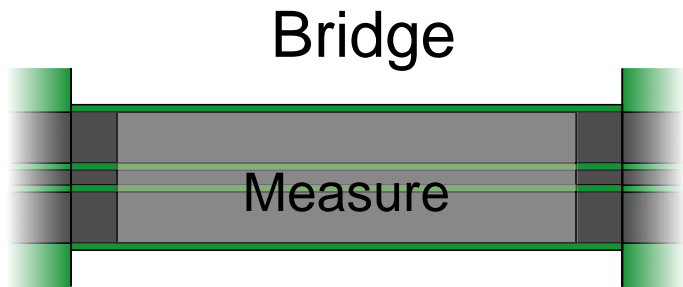
## Cantilever Sensors Detection of Nerve Gas



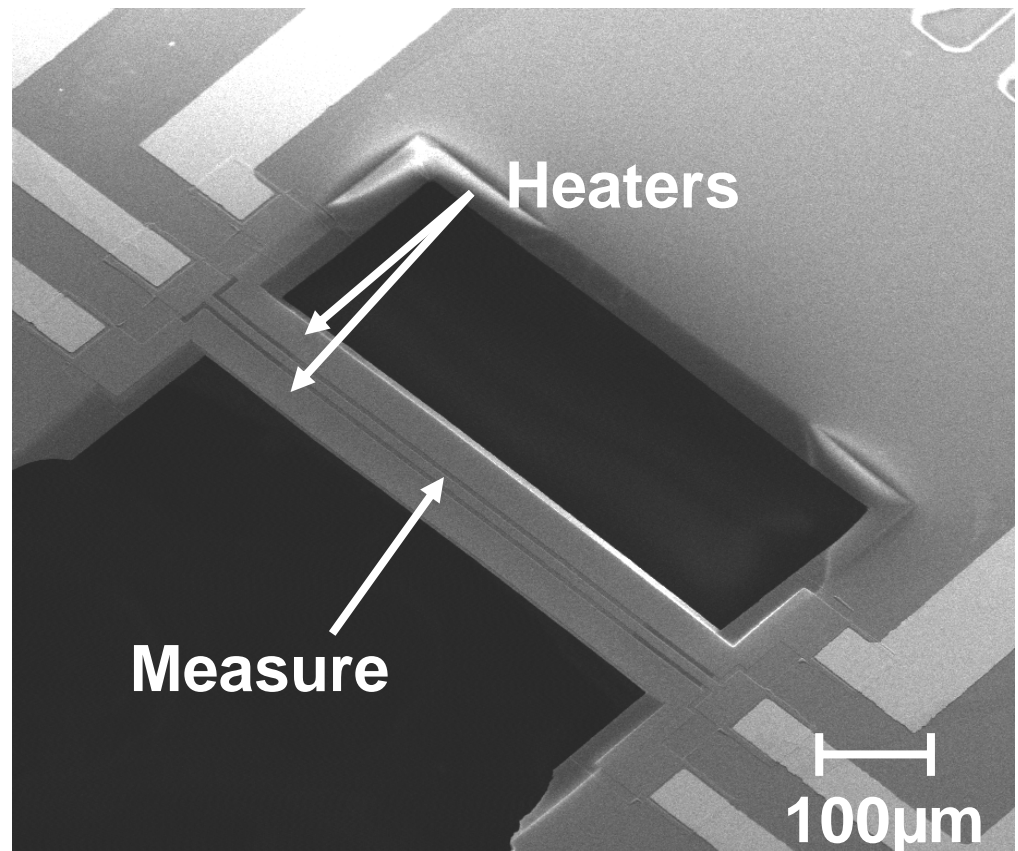
In collaboration with Lal Pinnaduwege, ORNL, USA  
The cantilever is coated with 4-mercaptopbenzoic acid (4-MBA) SAM

L.A. Pinnaduwege et al, Rev. Sci. Instrum. 78 (2007) 055101.

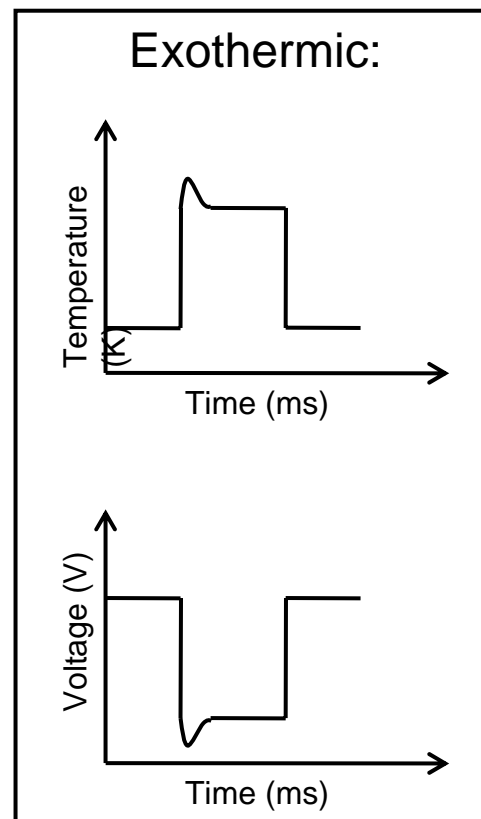
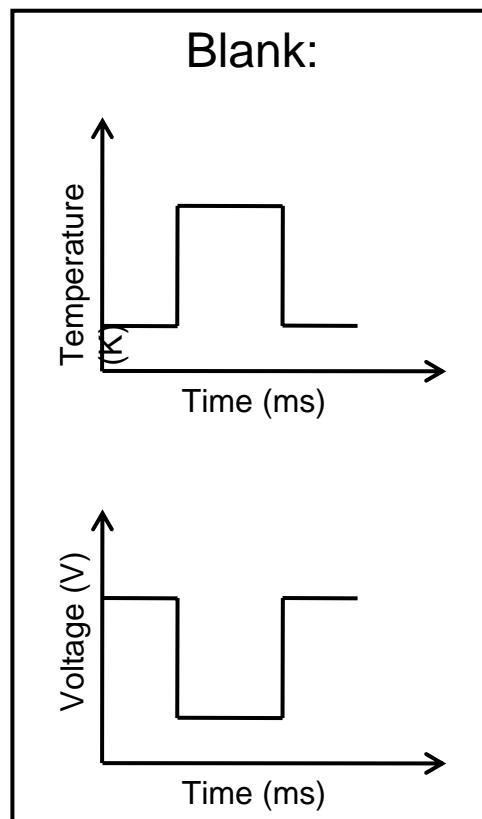
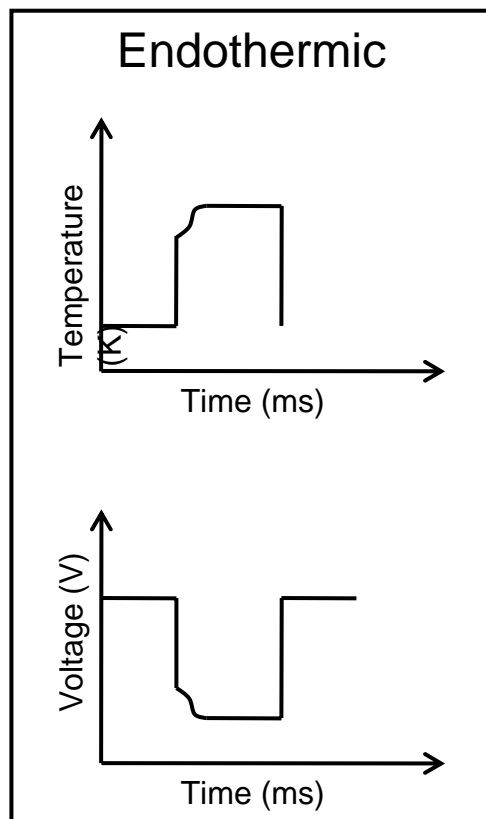
## Micro Calorimetric Sensors



SEM image:

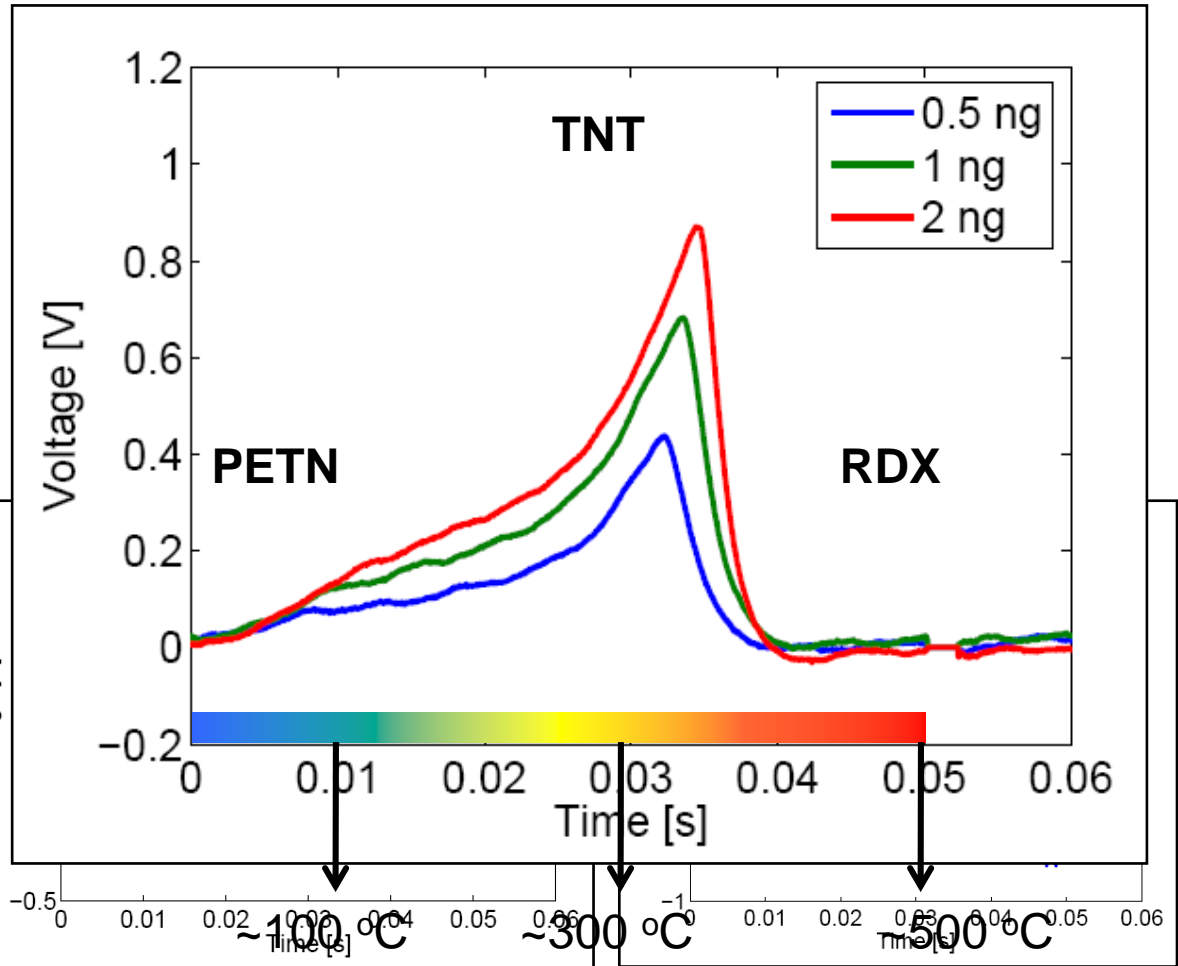
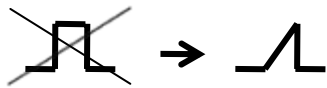


## Micro Calorimetric Sensors

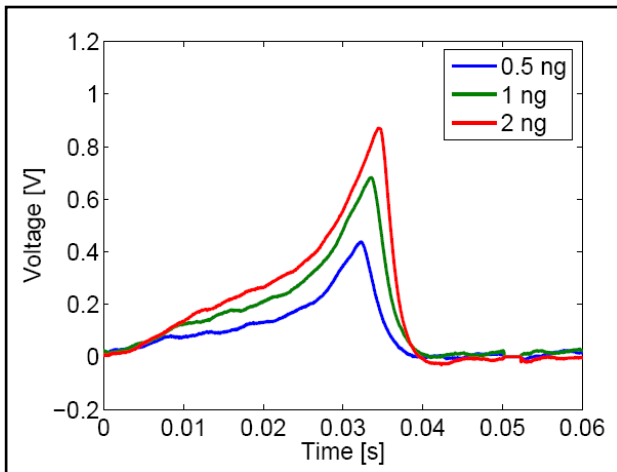


## Micro Calorimetric Sensors

Using a ramping pulse instead of a square heating pulse

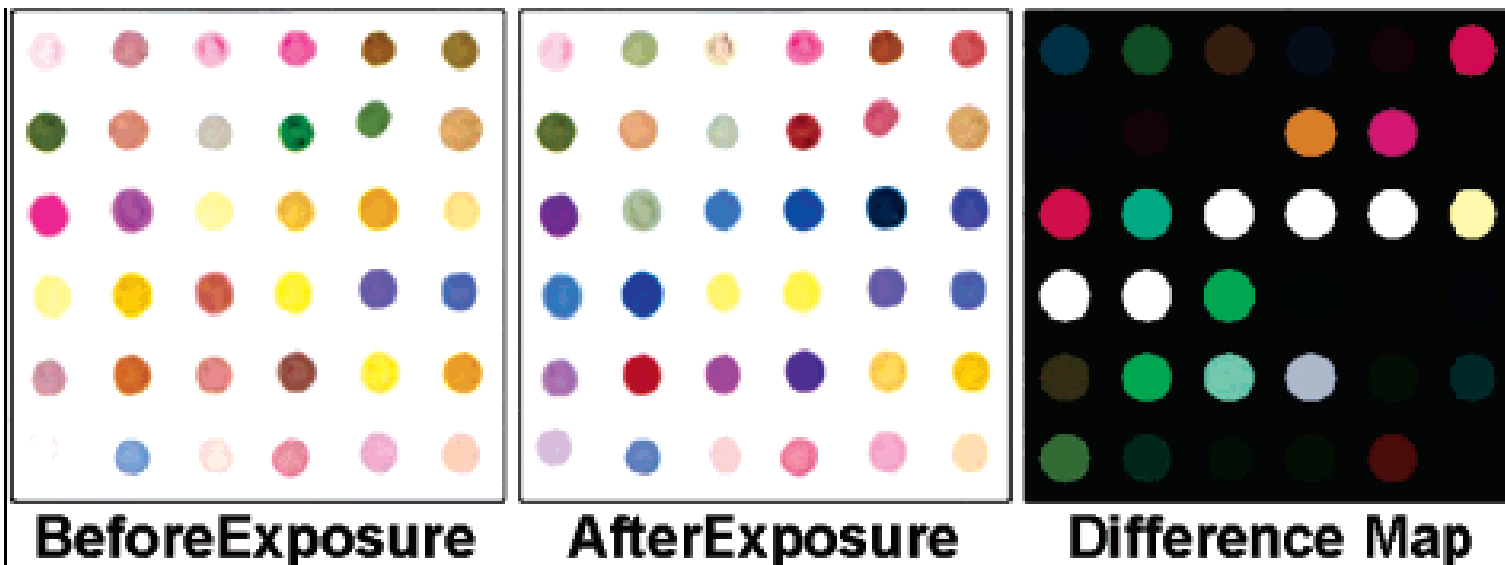


TNT





## Colorimetric Sensor Arrays



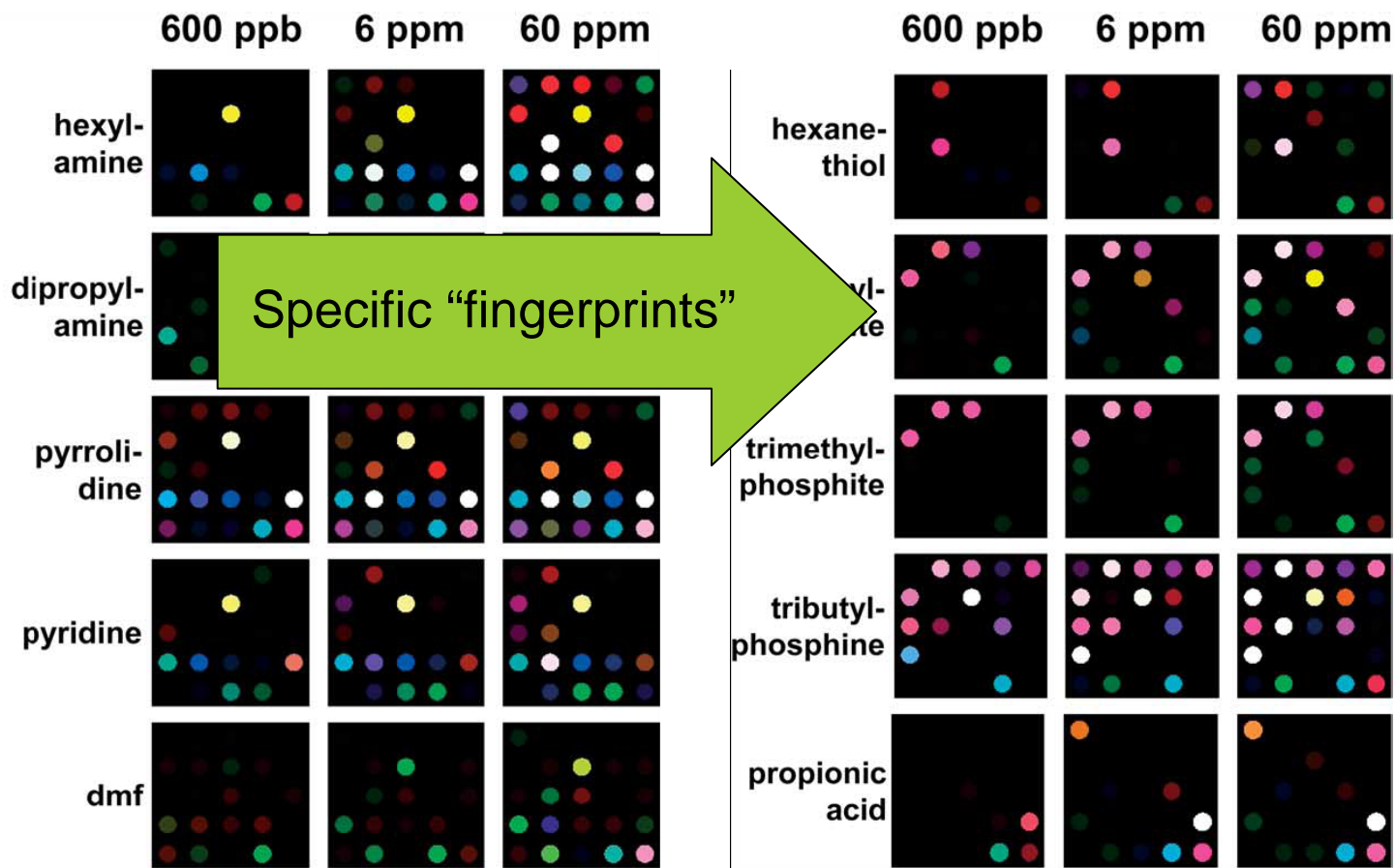
A colorimetric sensor array of chemoresponsive dyes

1. Before exposure to volatile organic compound (VOC)
2. After exposure
3. Color difference map

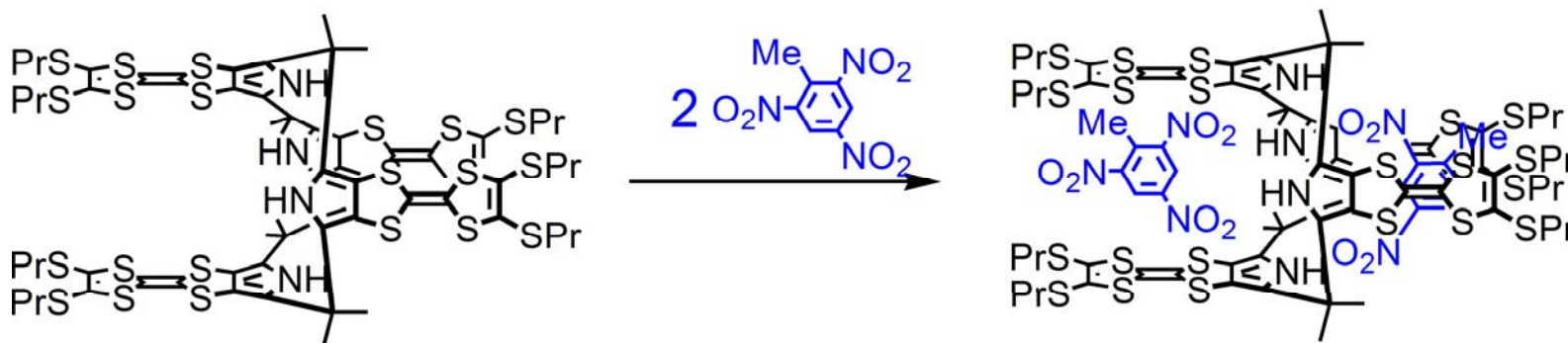




# Colorimetric Sensor Arrays



## Colorimetric Sensor Arrays



Jan O Jeppesen and Kent A Nielsen

Department of Physics and Chemistry  
University of Southern Denmark





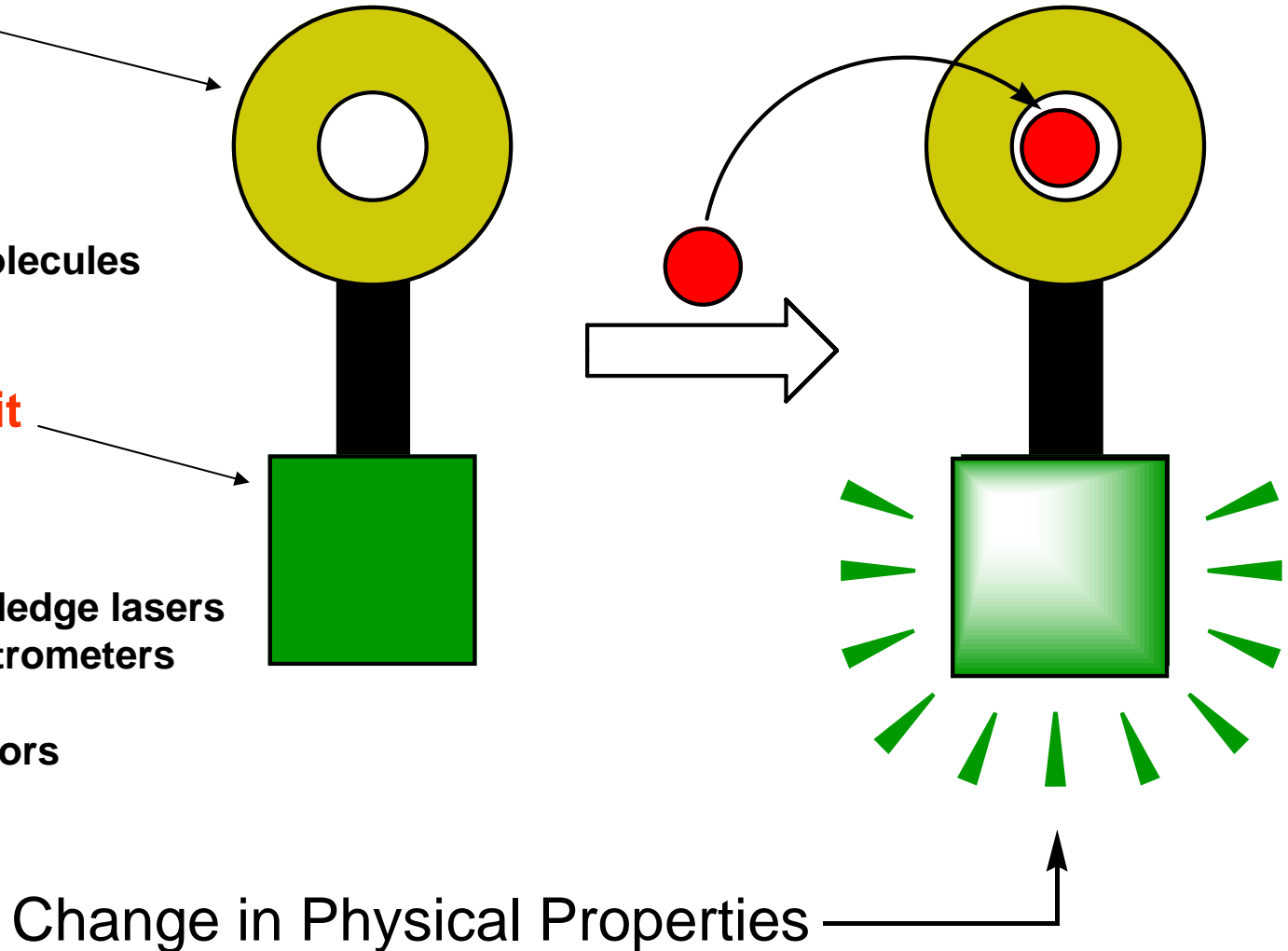
## Sensor Functionalization

### A Receptor Unit

- Antibodies
- Proteins
- Enzymes
- Peptides
- Chemoresponsive molecules
- Polymers

### A Transducer Unit

- Cantilevers
- Flappers
- Disc resonators
- Photonic crystal bandedge lasers
- Optical sensors/spectrometers
- SERS surfaces
- Electrochemical sensors
- Magnetic sensors



Change in Physical Properties



## Data Processing

- **Signal processing: optimal preprocessing of individual sensor data**
  - noise reduction
  - feature extraction
  - feature selection
- **Data and sensor fusion**
  - Learning based optimal nonlinear combination of sensor data
  - Outlier detection
  - Robustness against environment changes
  - Integration of context info
  - Time integration

Increased  
sensitivity

Increased specificity (lower false  
positive) and robustness/reliability

**Xsense**

**Thank you for your attention**