Wireless 3D Nanorod Composite Arrays based High Temperature Surface-Acoustic-Wave Sensors for Selective Gas Detection through Machine Learning Algorithms

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@ DOE Kick Off Meeting

Outline

- Objective/Vision
- Background
- Team Description and Assignments
- Task Descriptions
- Project Management Plan
- Conclusion and Outlook

Objective/Vision

- **Project Objective:**
  – The project objective is to develop a new class of wireless 3D nanorod composite arrays based high temperature surface-acoustic-wave gas sensors for selective and reliable detection through machine learning algorithms.

Background

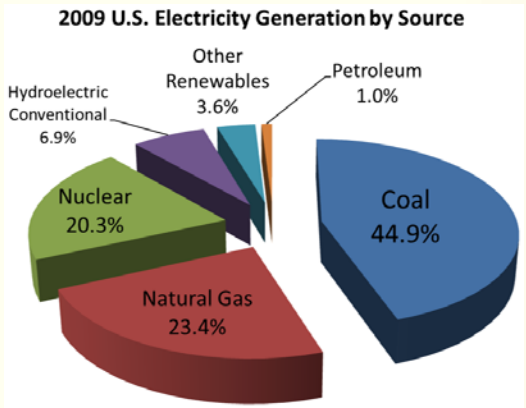
Importance of Harsh Environment Gas Sensors

➢ **Environment & Energy**

☺ Better control of **combustion**

☺ Reduce **emissions**

☺ Improve **energy efficiency**



Analysis based on 2008 coal costs and 2008 coal-fired power plant fleet (units greater than 300 MW)

1% Improvements/increases are easily achievable by advanced sensors and controls.

Coal Consumed

35,700 MMBTU/yr

$70 Million/yr

@ $2/MMBTU

Power Generated

3.5 Billion kWh/yr

@ 80% capacity factor

➢ **Entire coal-fired fleet**

1% EFFICIENCY improvement

- $300 million/yr coal cost savings
- Reduction of 14.5 million metric tons CO_2 per year

1% increase in AVAILABILITY

- More than 2 GW of additional power from existing fleet

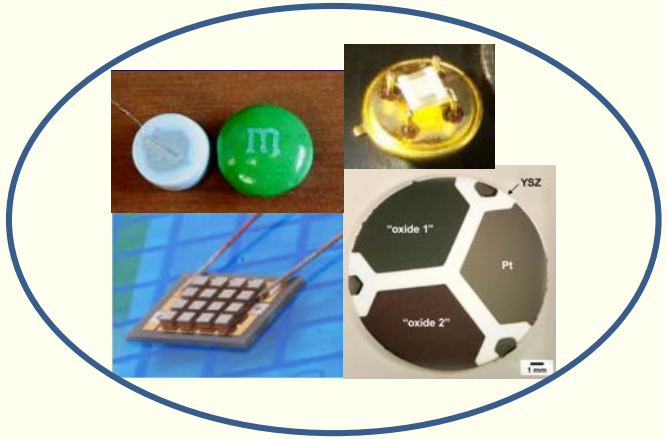
* NETL Sensors and Controls Program Overview, 2012.

Background

Sensors for Harsh Environments

Solid Oxide Fuel Cells
- 650 – 1000 ^{o}C
- Atmospheric pressure

Advanced Combustion Turbines
- Up to 1300 ^{o}C combustion temperatures
- Pressure ratios of 30:1



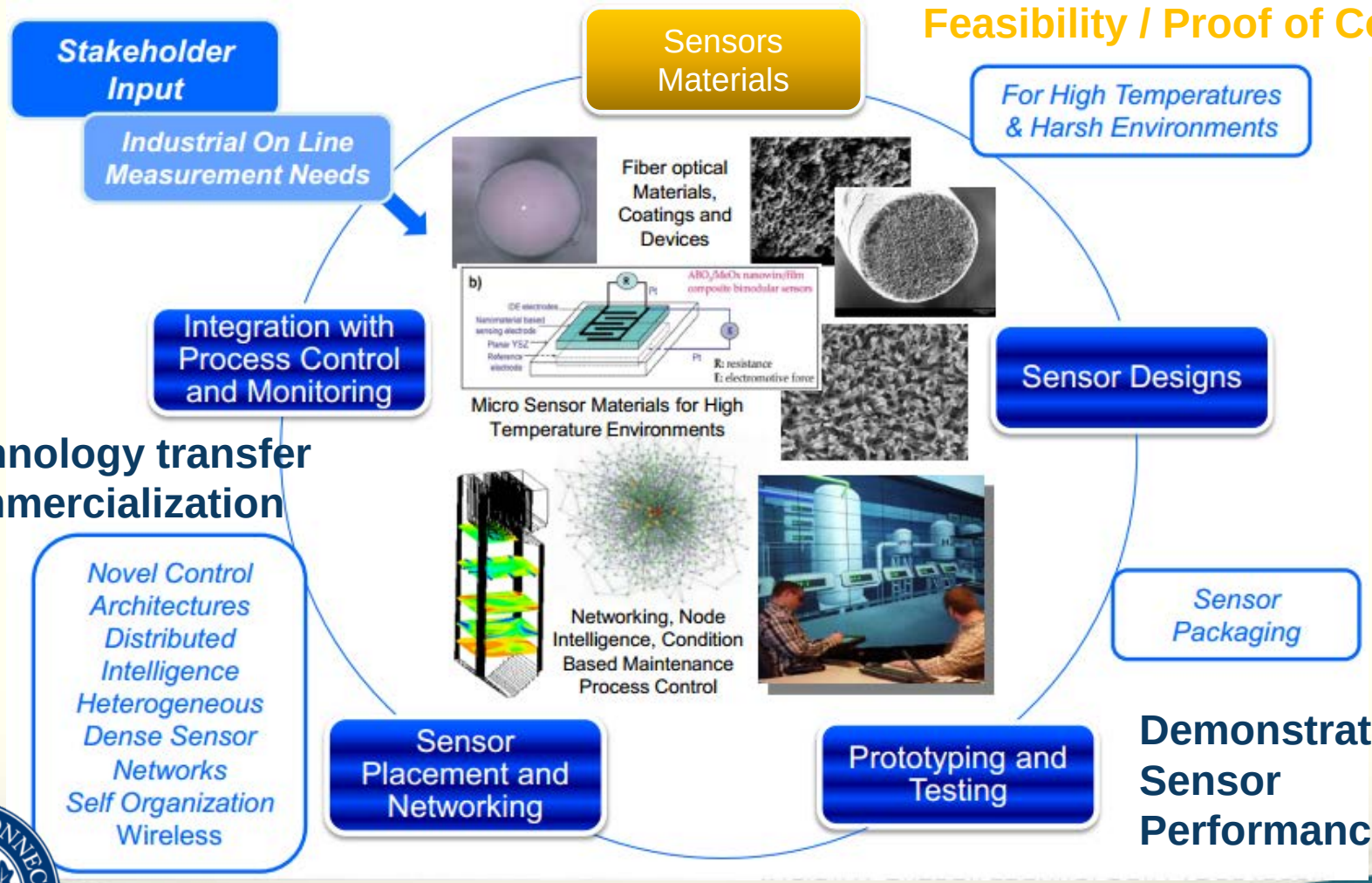
Automotive Engine
- up to 1000 ^{o}C
- Compression ratio ~10:1

Ultra Supercritical Boilers
- Up to 760 ^{o}C temperature
- Up to 5000 PSI pressure

Gasifiers
- Up to 1600 ^{o}C, and 1000 PSI (slagging gasifiers)
- Erosive, corrosive, highly reducing environment

Background

Research in Sensors and Controls



* NETL Sensors and Controls Program Overview, 2012.

Background

Current Solid-State Sensing Technologies

Potentiometric

- Commercialized O_2 sensor (Zirconia)
- CO_2, SO_x (K_2CO_3, Ag_2SO_4) at mild T

Amperometric

- Diffusion limited current (linear)
- O_2, H_2, CO, NO_x, SO_2, H_2S

Mixed Potential

- Thermodynamic non-equilibrium
- More than one electrochemical reaction occurs
- The oxidation and reduction reactions are for different species
- CO, NO_x, HCs in 500 – 600 ^oC

Resistive

- **Bulk conduction-based**
  O_2 at 700 – 1100 ^oC
- **Surface conduction-based**
  CO, HCs, H_2, NO_x in 200 – 500 ^oC
- **Metal/oxide junction based**
  MS/MIS, MOSFET, Schottky diodes

Impedancemetric

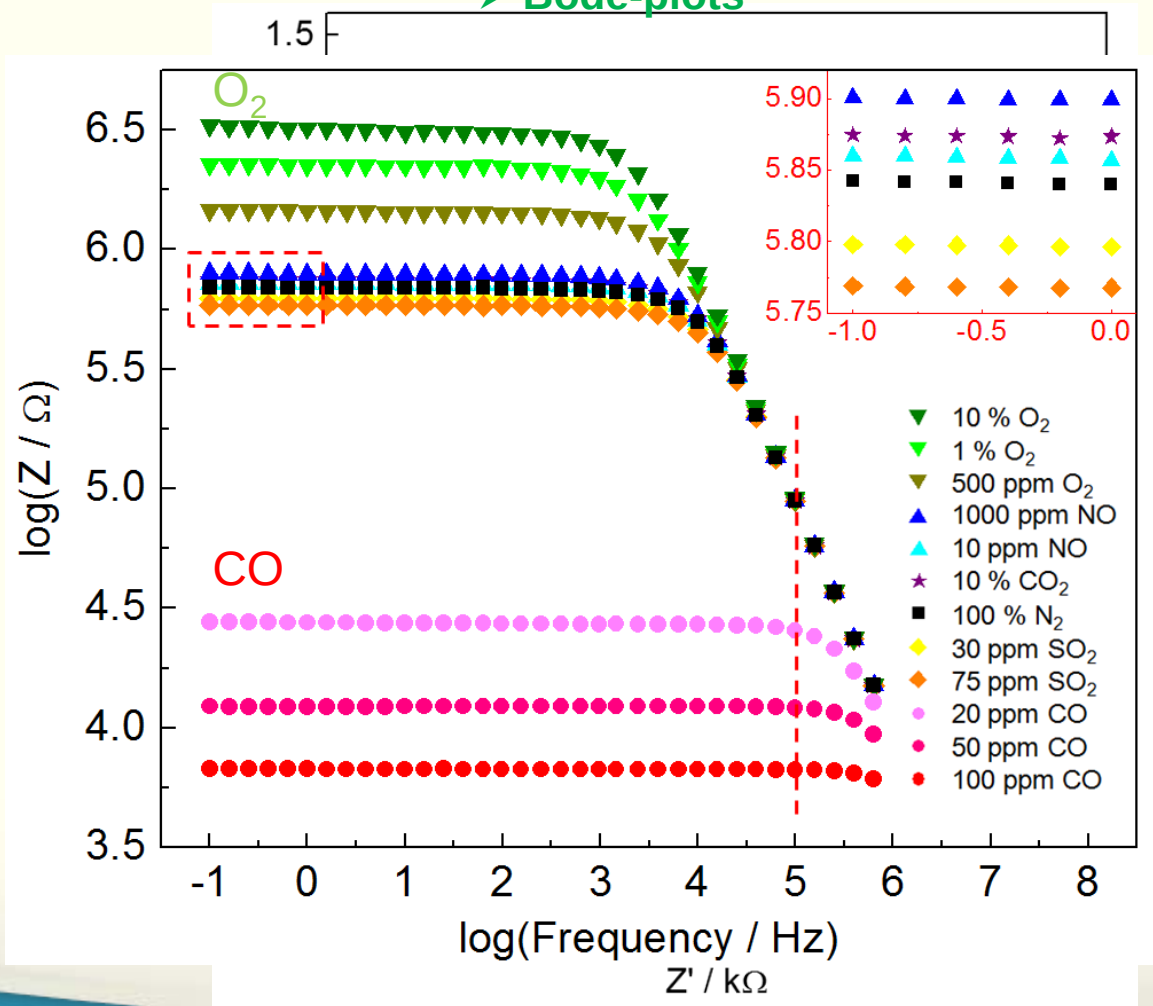
- AC measurements at a specified F
- Solid-electrolyte or resistor configured
- H_2O, CO, HCs, NO_x
- Measure total NO_x concentration
- Accurate detection on single ppm level

* **Yixin Liu**, et al., Solid-State Gas Sensors for High Temperature Application - A Review, *J Mater. Chem. A*, 2014, **DOI:** 10.1039/C3TA15008A

Pt-CeO_2 NFs Impedancemetric Based Sensor

Impedance Spectra

- Nyquist plots
- Bode-plots

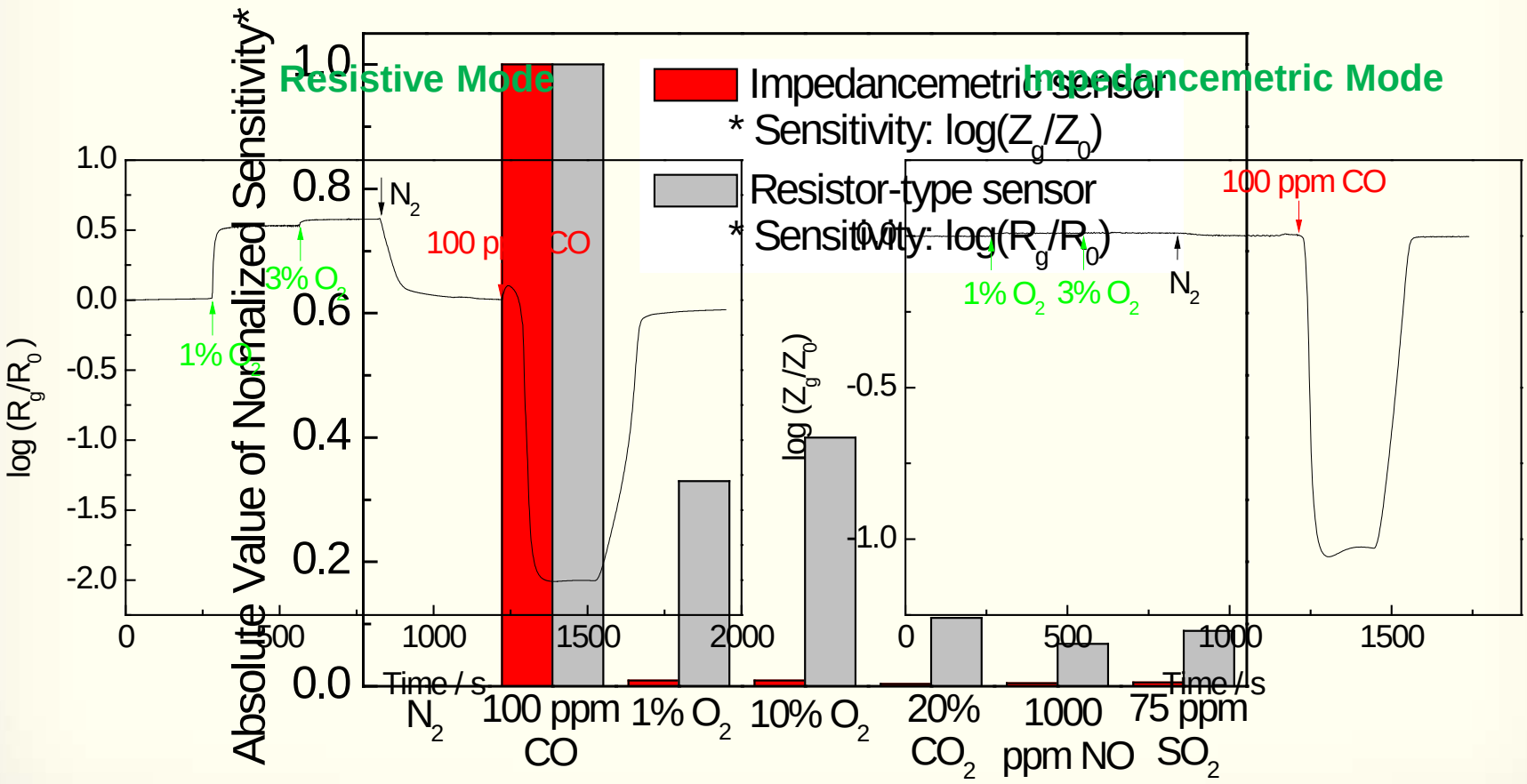


- Initial potential: 0 V
- Amplitude: 0.5 V

* **Yixin Liu** and Y. Lei, Pt-CeO_2 nanofibers based high-frequency impedancemetric gas sensor for selective CO and C_3H_8 detection in high-temperature harsh environment, *Sens. Actuators B*, 2013, 188, 1141-1147.

Pt-CeO_2 NFs Impedancemetric Based Sensor

Improved Selectivity at High Frequency



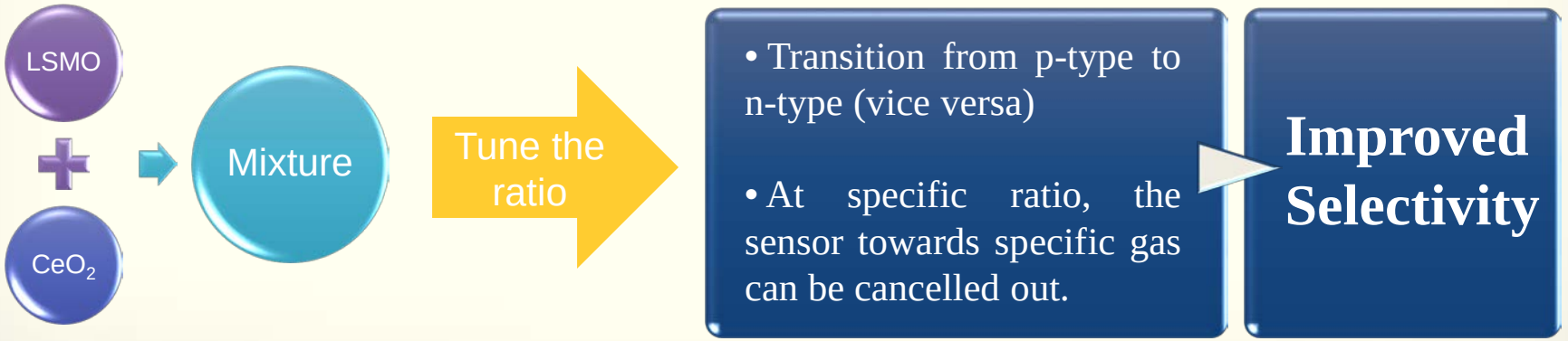
p-LSMO/n-CeO_2 NFs heterojunction Based Sensor

Rationale

❖ **Properties of LSMO (p-type) and CeO_2 (n-type)**

Material	Type	Charge carrier	Resistance	In reducing gas	In oxidizing gas
LSMO	p-type	Holes	Low	R ↑	R ↓
CeO_2	n-type	Electrons	High	R ↓	R ↑

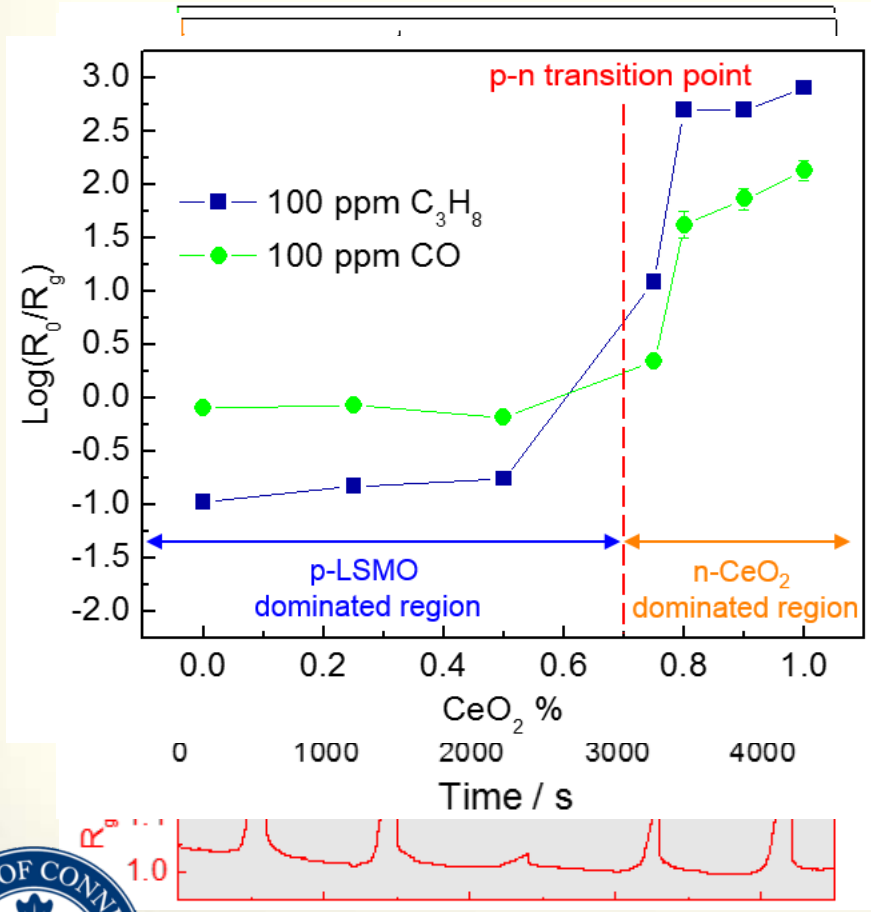
❖ **Rationale**



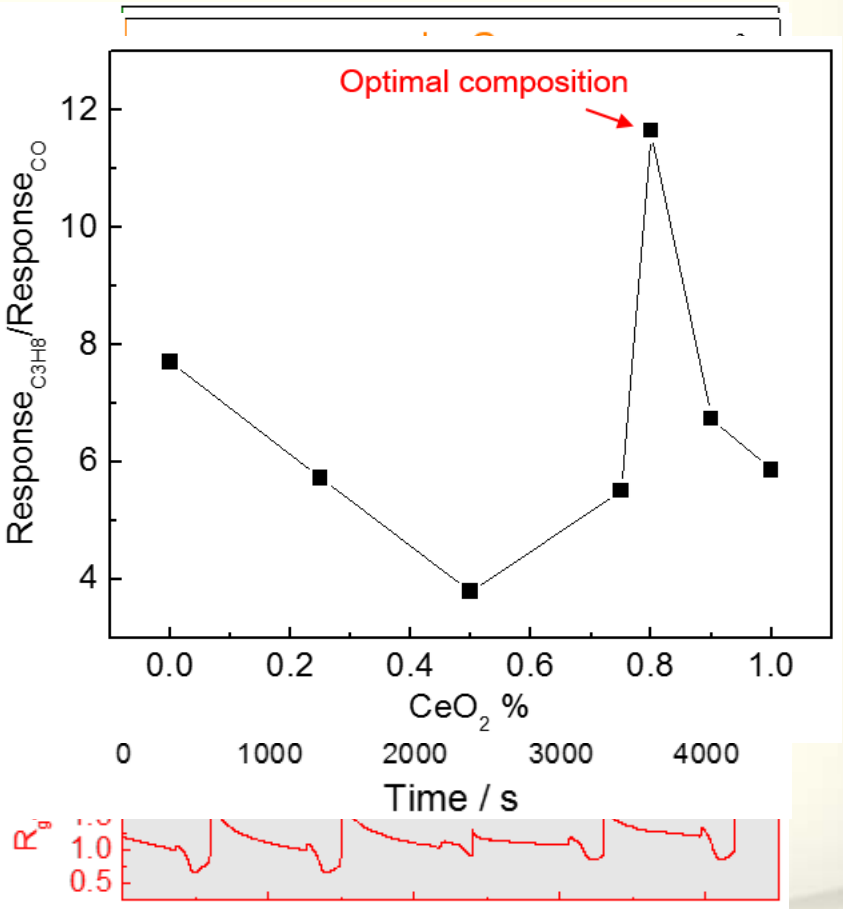
p-LSMO/n-CeO_2 NFs heterojunction Based Sensor

Systematic Study of Sensing Performance

CO detection

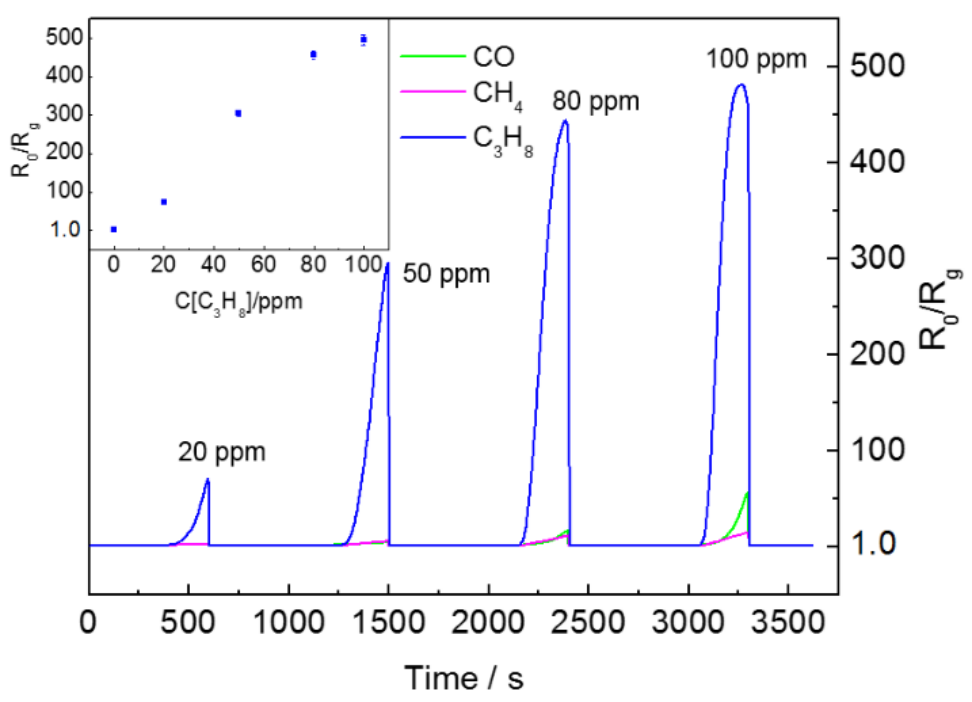


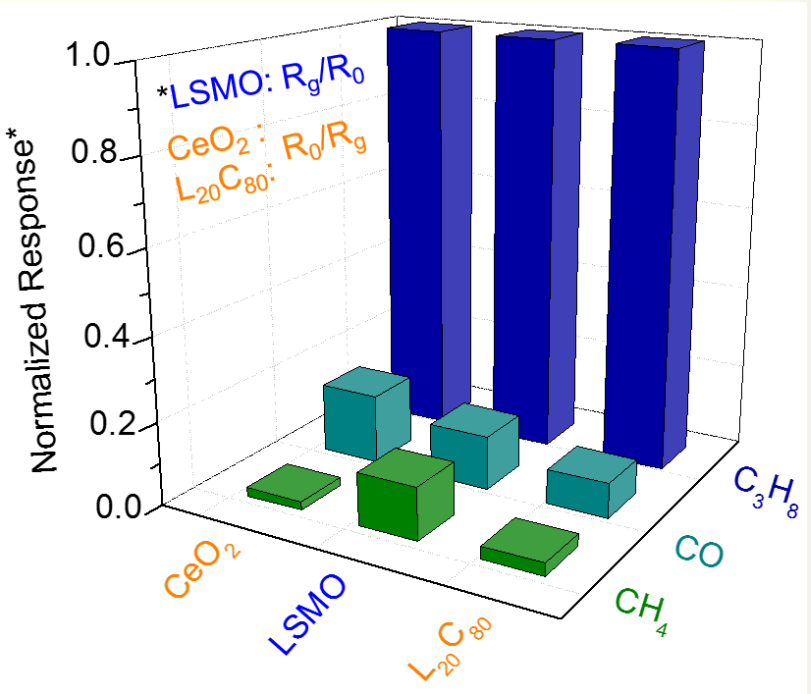
Propane detection



p-LSMO/n-CeO_2 NFs heterojunction Based Sensor

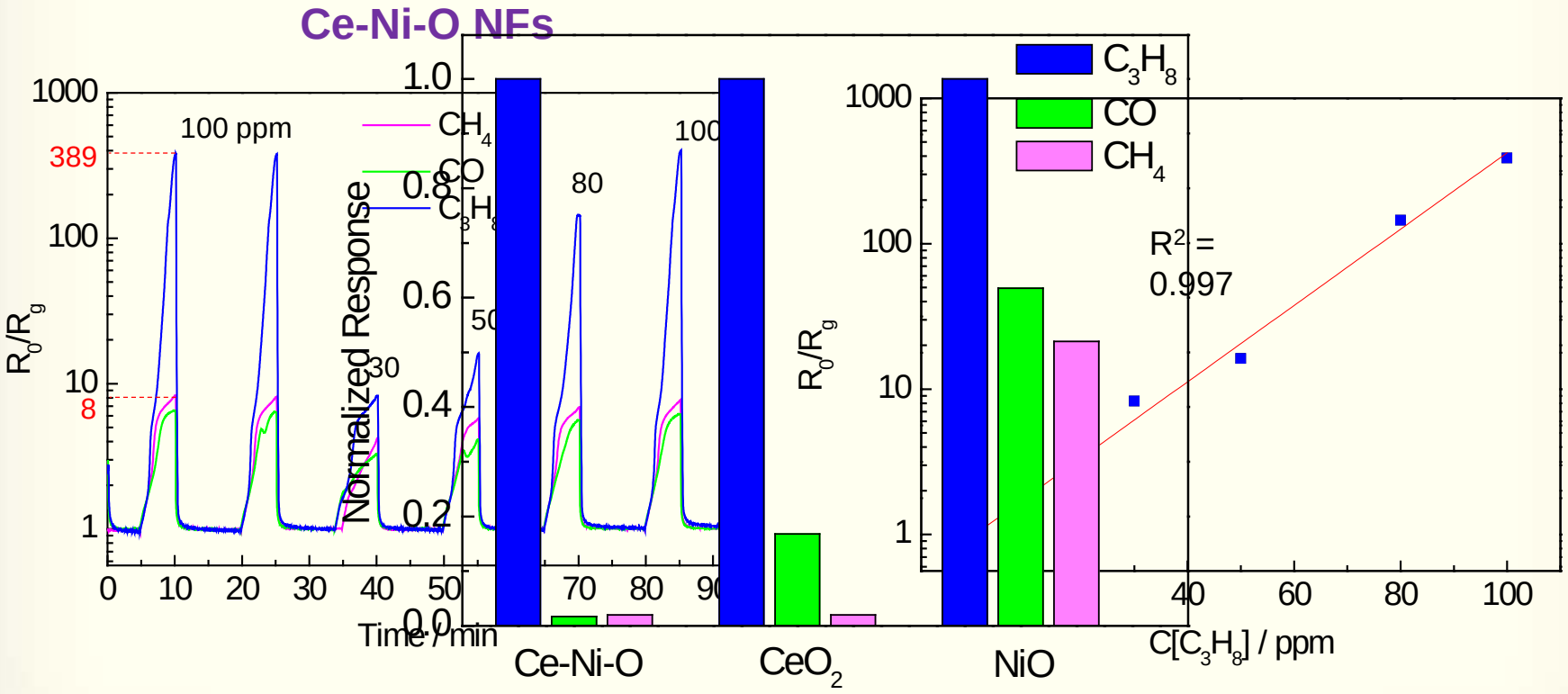
Real-Time Detection on $L_{20}C_{80}$ – Based Sensor





Ce-Ni-O NFs Based Sensor

Gas Sensing Performance



Backgound

- Wireless monitoring and Selectivity are the most pressing issues in high temperature gas sensing field
- Urgent need to develop gas sensors to achieve highly selective and wireless detection of gas species and concentration in high-temperature mixed gases environment

Team Description and Assignment

- PI Yu Lei, Castleman Associate Professor, UConn Chemical Engineering (ChE) – an expert in the metal/metal oxide synthesis, chemical sensor design and testing, and microfabrication
- Co-PI Pu-Xian Gao, Associate Professor, UConn Materials Science and Engineering (MSE) – an expert in 3D nanomaterials architecture design, assembly, fabrication, characterization, and applications.
- Co-PI Sanguthevar Rajasekaran, UTC Chair Professor and Director of the Booth Engineering Center for Advanced Technologies (BECAT), UConn Computer Science and Engineering (CSE) – an expert in the areas of Applied Algorithms, Bioinformatics, Biomedical Informatics, High Performance Computing

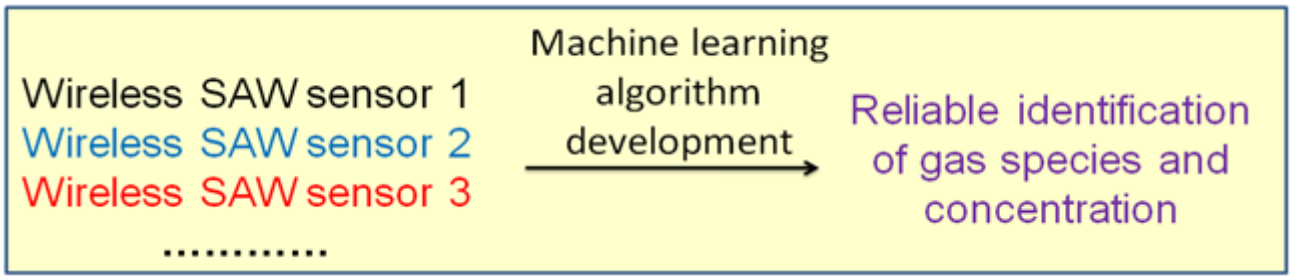
Team Description and Assignment

- **PI Yu Lei group – develop wireless SAW device and conduct gas sensing detection.**
- **Co-PI Pu-Xian Gao group – fabricate high temperature stable nanorods and material characterization**
- **Co-PI Sanguthevar Rajasekaran group – develop machine learning algorithms**

Task Desciptions

- Design and fabrication of passive wireless surface-acoustic-wave (SAW) arrays
- In-situ growth of nanorods sensing materials
- Structural and thermal stability characterizations of nanorod composites
- Test the wireless 3D nanorod composite SAW sensor arrays and develop machine learning algorithms
- Validate the wireless 3D nanorod composite SAW sensor arrays with integrated machine learning algorithms for monitoring methane combustion process in lab environment.

Task Desciptions



Project Management Plan

- Dr. Yu Lei, as the PI, will ensure that the individual activities meet goals on time and within budget.

- The project as a whole will be managed by Dr. Lei with an eye toward effective communication of accomplishments and results to the DOE/NETL.

- Project reports, technical presentations, and other publications will be prepared to disseminate information.

Conclusions and Outlook

High temperature gas sensors working in harsh exhaust environment are of paramount importance to improve combustion efficiency and control emissions.

In our past 7-year work on high temperature gas sensor, we have achieved good thermal **Stability** and **Sensitivity.**

By combining the concept of high-temperature stable passive wireless SAW sensor arrays with novel high-temperature stable perovskite coated three-dimensional (3D) metal oxide nanorod composites as well as machine learning algorithms, we expect to achieve highly selective and wireless detection of gas species and concentration in high-temperature mixed gases environment.

Acknowledgement

- Thank the supporting from Department of Energy.

Thank You !

Questions ?