
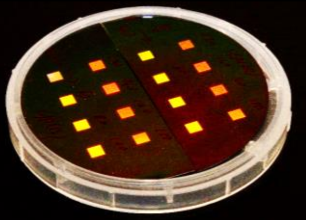
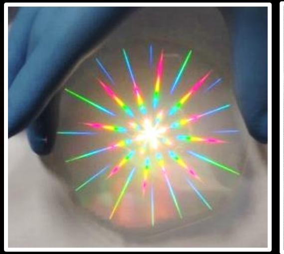
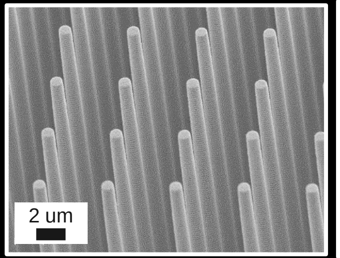

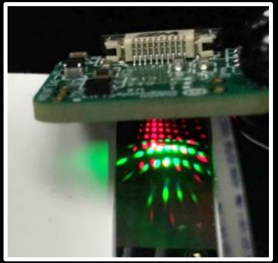
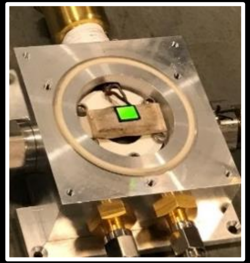

Exploring Natural and Bio-inspired Photonic Nanostructures as Gas Sensors:

From Scientific Curiosity to Unexpected Discoveries and to Societal Impact

Radislav A. Potyrailo
GE Vernova Advanced Research Center

IEEE MEMS & Sensors SFBA Chapter Meeting
October 2, 2024

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May 4-7, 2025

IEEE APSCON 2025

IEEE Applied Sensing Conference

Hyderabad, India
January 20-22, 2025

IEEE BIOSENSORS 2025
SAN DIEGO, CA, USA || AUGUST 2-5, 2025

IEEE BioSensors Conference

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IEEE Conference on Agrifood Electronics

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Sensor Interfaces Meeting

IEEE Sensor Interfaces Meeting

Veldhoven, Netherlands
May 12-13, 2025

Sensors in Spotlight

IEEE Sensors in Spotlight

Boston, MA, USA
May 9, 2025

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- Impact factor 4.325

IEEE Sensors Letters

- Established in 2017
- Rapid publication of short papers

Co-Sponsored Publications

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- IEEE Internet of Things Journal
- IEEE Trans. on Agrifood Electronics
- IEEE Journal of Indoor and Seamless Positioning and Navigation
- IEEE Trans. on Radar Systems
- IEEE Trans. on Big Data
- IEEE Trans. on GAMES

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- Published quarterly
- Reach of over 25,000 subscribers

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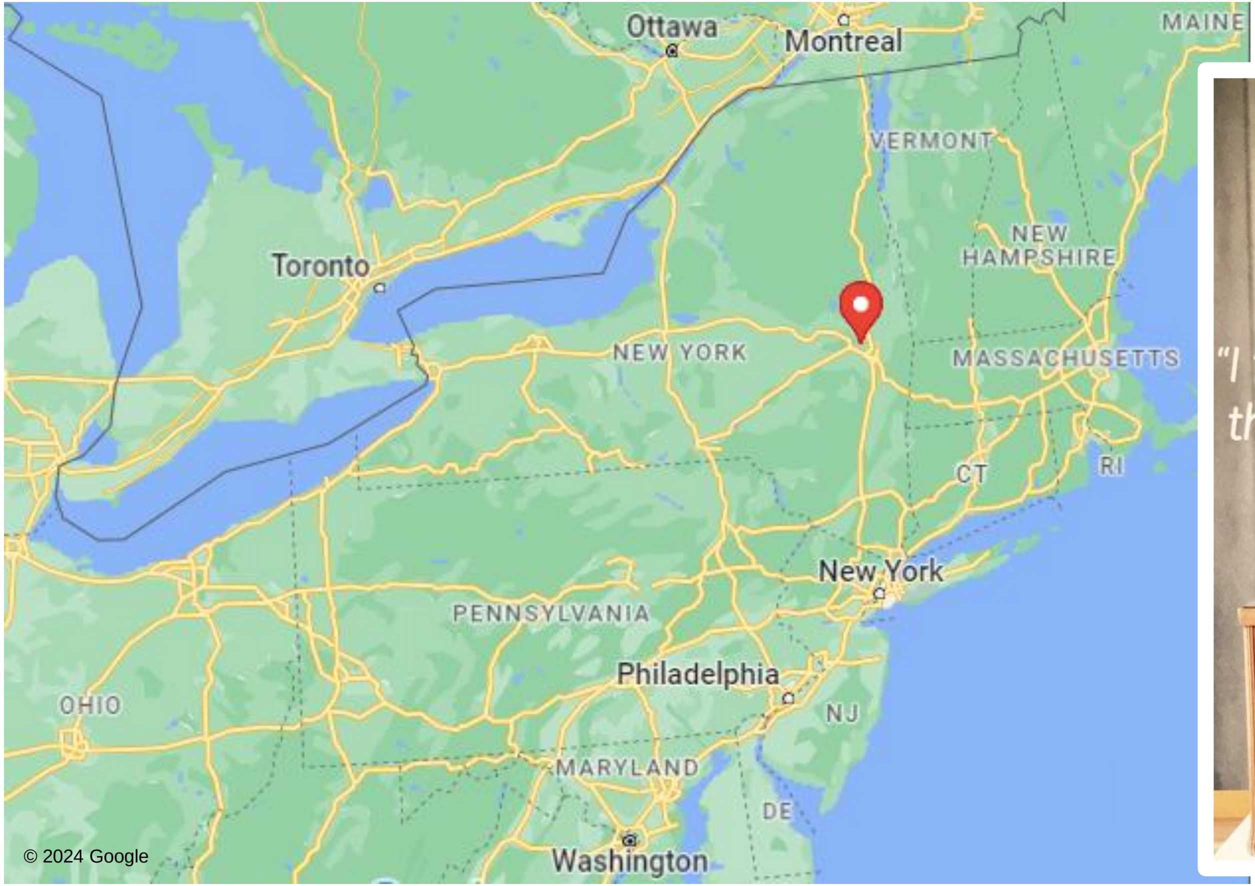
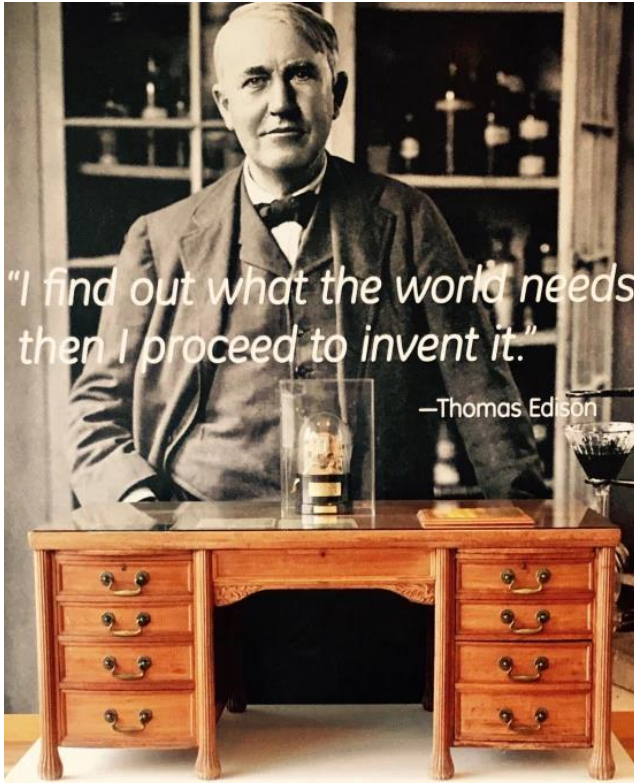




GE Vernova portfolio of businesses

Diverse topic areas of R&D interest of GE Vernova Advanced Research Center:

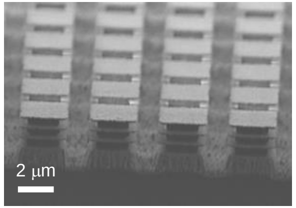
- Next generation multi-parameter monitoring and prognostics solutions of critical industrial assets
- Reductions in greenhouse gas emissions (including CO2, CH4, N2O, HFCs, H2)
- Fuel cells, batteries, and energy storage
- Carbon capture, utilization, and storage
- Processes that enhance industrial efficiency, building construction/maintenance efficiency
- Production of clean energy including solar, hydrogen, nuclear, or other clean energy sources

Lecture outline:
Learning from *Nature*

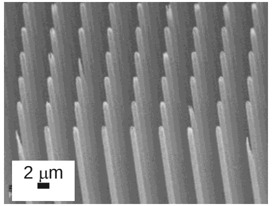
Toward Societal Impact

Bioinspiration – new functionality, beyond Nature

High temp. sensing



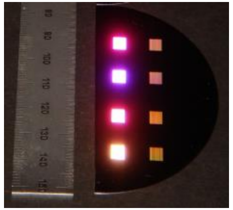
Aspect ratio 93:1

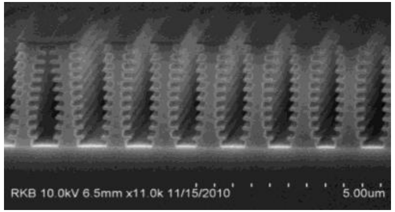


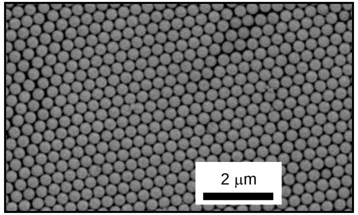
Multivariable fiber-optics

Biomimetics – recreation of observed functionality

Multi-gas sensing at room temperature

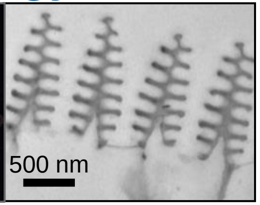






Understanding Status Quo of conventional gas sensors

Biology



GE VERNOVA IEEE Sensors Council

Every century – solving practical gas-detection challenges

World War I soldiers as gas scouts

https://www.hsdl.org/?view&did=1670

Alcohol levels in breath

http://garda-post.com/breathalyser-testing-a-brief-history/

Canaries in mines per safety regulations

http://news.bbc.co.uk/

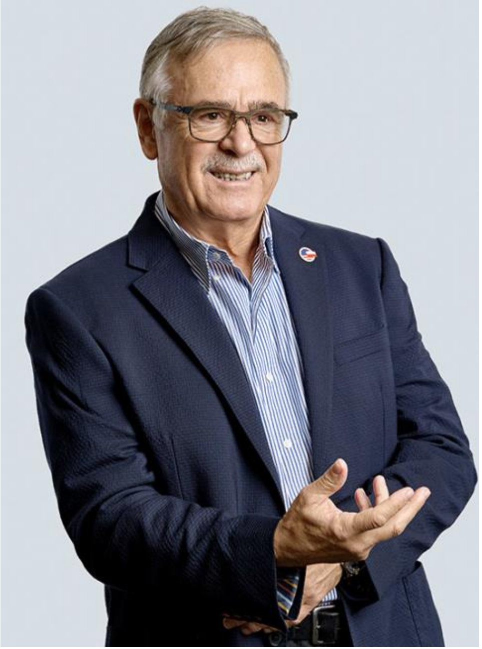
http://ae.msasafety.com/msa100

20th century:
Security and industrial safety needs and demands drive practical available solutions

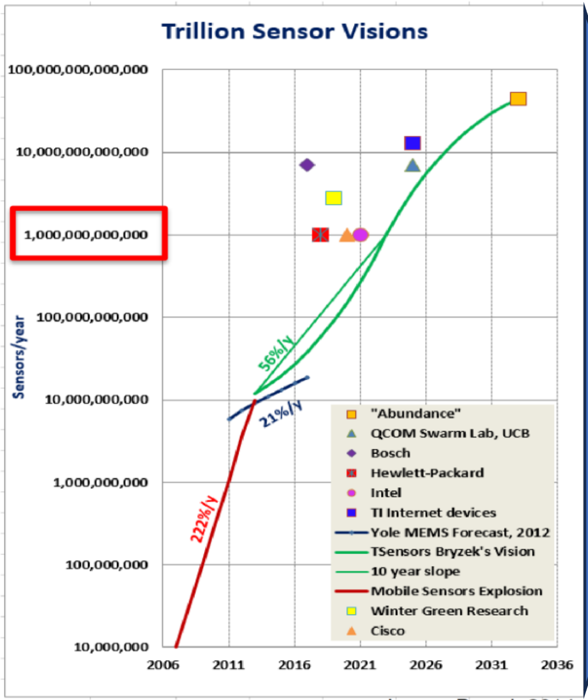
Trillion Sensor Universe

Bryzek, J., *Roadmap for the Trillion Sensor Universe*.
International Electronics Manufacturing Initiative Spring Member Meeting and Webinar: Berkeley, CA, **2013**

Dr. Janusz Bryzek



https://www.exo.inc/our-people/janusz-bryzek



Janusz Bryzek 2014

Dec. 8, 2022

PETER H. DIAMANDIS

METATREND #9: TRILLION-SENSOR ECONOMY: THE ABILITY TO SENSE AND KNOW ANYTHING, ANYTIME, ANYWHERE

https://www.diamandis.com/blog/metatrend_9_trillion_sensor_economy

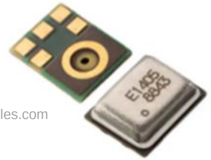
High demand for high-quality sensors

Sensors for mobile applications: annual sales of billions of units

Pressure sensors

www.st.com

Microphones



www.knowles.com

Accelerometers

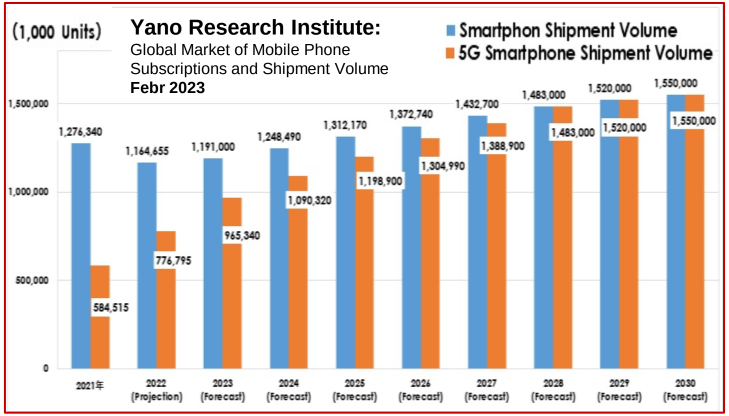
www.nxp.com

Compasses

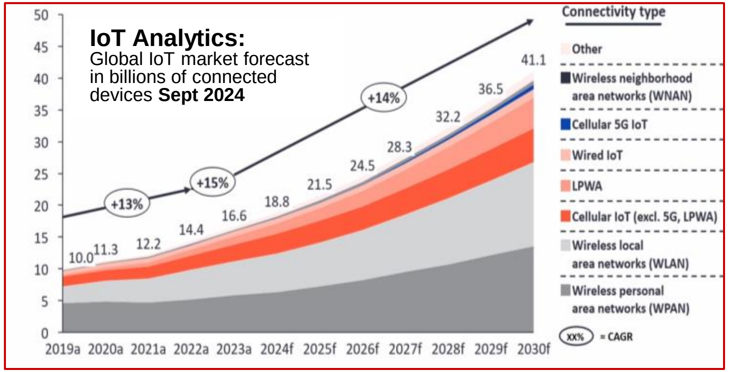
www.st.com

Gyroscopes

www.bosch-sensortec.com



https://www.yanoresearch.com/en/press-release/show/press_id/3180



https://iot-analytics.com/number-connected-iot-devices/

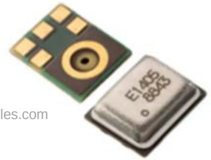
High demand for high-quality sensors

Sensors for mobile applications: annual sales of billions of units

www.st.com

Pressure sensors

Miniaturization into wearables
Sensor fusion at chip level
AI-driven analytics



www.knowles.com

Microphones

Improved active noise cancellation
Wider dynamic range
Advanced beamforming

www.nxp.com

Accelerometers

Miniaturization into wearables
Advanced signal conditioning
Sensor fusion

www.st.com

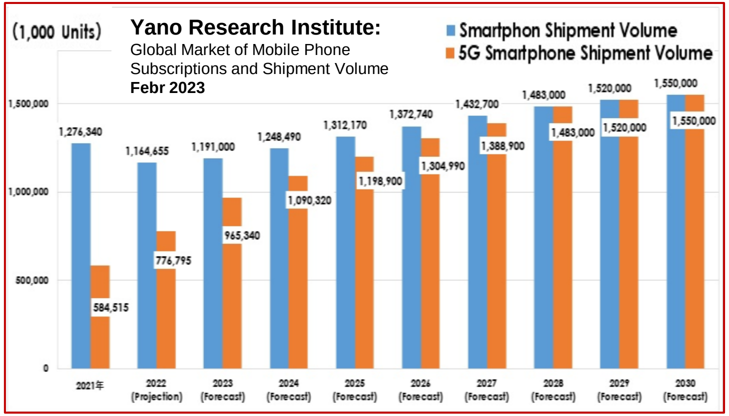
Compasses

Reduced magnetic interferences
Wider dynamic range
Built-in control logic

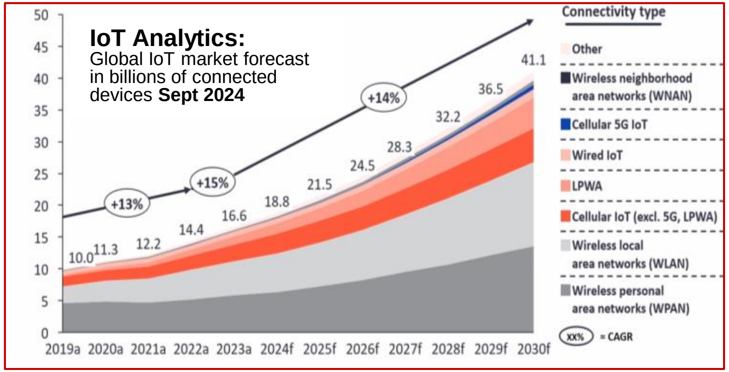
www.bosch-sensortec.com

Gyroscopes

Miniaturization into wearables
Lower drift rates
Sensor fusion



https://www.yanoresearch.com/en/press-release/show/press_id/3180

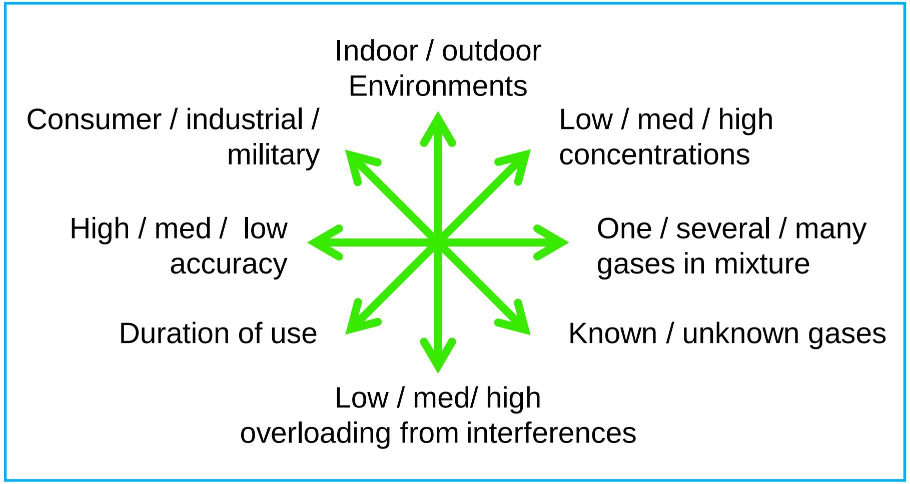


https://iot-analytics.com/number-connected-iot-devices/

Enhanced performance capabilities lead to increased demand for sensors

Modern gas sensors:
Diverse requirements for myriad applications

- **Safety**
- **Security**
- **Regulations**
- **Productivity**
- **Convenience**
- **Comfort**
- **Etc...**



Understanding diverse requirements for myriad applications of modern gas sensors

Top ten requirements

- High accuracy
- High selectivity
- Broad dynamic range
- Low initial cost
- Low operation cost
- Low power consumption
- Fast response time
- High sensitivity
- Small size
- High stability

Top five requirements

- High reliability/ accuracy
- Low cost
- Low power
- Standard communication
- Data security

Top three requirements

- High reliability/ accuracy
- Low cost
- Low power

Potyrailo, Mirsky, *Chem. Rev.* **2008**
Potyrailo et al., *Chem. Rev.* **2011**
Potyrailo, Naik, *Annu. Rev. Mater. Res.* **2013**
Potyrailo, *TSensors Summit* **2015**

Markets for Sensors in Industrial Internet, **2014**
Potyrailo, *IEEE SENSORS* **2018**
Potyrailo, *IEEE SENSORS* **2022**
Potyrailo, *IEEE SENSORS* **2023**
Potyrailo, *ISOEN* **2024**

Needs for hydrogen sensors in diverse applications

Table from: *Nature Materials*, *18*, **2019**, 489–495

Parameter	Performance Requirement		
	Stationary Systems*	**Automotive Systems****	**Safety Systems*****
Measurement Range	up to 4%	up to 4%	0.1% - 10%
Detection Limit	< 100 ppm	-	-
Operating Temperature	-20 ^{0}C – 50 ^{0}C	-40 ^{0}C – 125 ^{0}C	-30 ^{0}C – 80 ^{0}C
Response Time	< 30 s	< 3 s	< 1 s
Recovery Time	< 60 s	< 3 s	-
Accuracy	25%	-	5%

* ISO 26142:2010 Hydrogen detection apparatus - Stationary applications **2010**

** U.S. Dept of Energy, Hydrogen, Fuel Cells & Infrastructure Technologies Program. Multi-Year Research, Development, and Demonstration Plan, 2003-2010. Section 3.4 Fuel Cells. **2005**

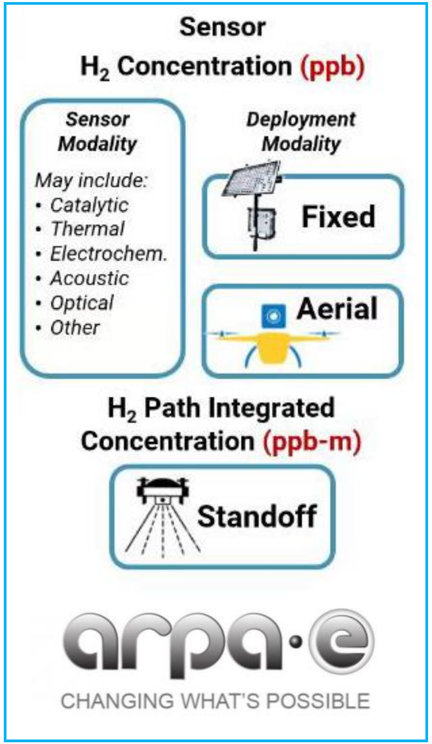
*** U.S. Dept of Energy, Energy Efficiency and Renewable Energy (EERE). Multi-Year Research, Development, and Demonstration Plan, 2011-2020. Section 3.7 Hydrogen Safety, Codes and Standards **2015**

https://medium.com/@imirsanket7/hydrogen-fueling-station-market-size-status-ongoing-trends-and-forecast-to-2031

https://fuelcellsworks.com/news/airbus-fine-tunes-hydrogen-decision-schedule/

https://www.powermag.com/content-collection/top-plant-successful-green-hydrogen-demonstration-project-is-a-step-toward-a-carbon-free-future/

2024



https://arpa-e.energy.gov/technologies/exploratory-topics/H2SENSE

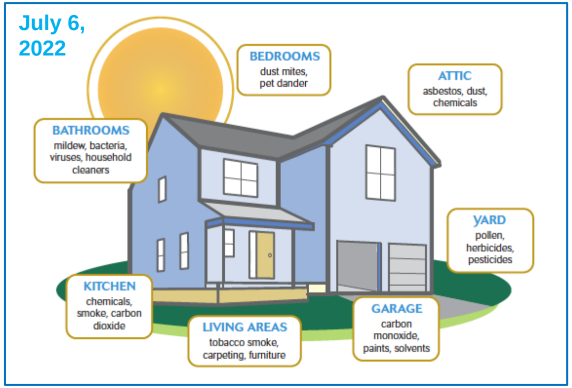
Illustrative types and safe levels of indoor volatiles

Chemical Substance	EPA, USA (8 hours daily)	DFG, Germany (8 hours daily)	WHO (exposure time)
Benzene	29 mg/m³	0.2 mg/m³	No safe level
Formaldehyde	1.12 mg/m³	0.37 mg/m³	0.1 mg/m³ (30 min)
Napthalene		0.5 mg/m³	0.01 mg/m³ (1 year)
Styrene	86 mg/m³	86 mg/m³	0.26 mg/m³ (1week)
Trichloroethylene	420 mg/m³	33 mg/m³	230 mg/m³ (lifetime risk of 1/10.000)
Tetrachloroethylene	241 mg/m³	138 mg/m³	0.25 mg/m³ (1 year)
Toluene	257 mg/m³	190 mg/m³	0.26 mg/m³ (1 week)

https://www.catsensors.com/media/Decentlab/Productos/IAM_interior/Overview_TVOC_and_IAQ.pdf


Science
March 28, 2024
BACK TO VOL. 383, NO. 6690
DOI: 10.1126/science.adl0677
POLICY FORUM | PUBLIC HEALTH
Mandating indoor air quality for public buildings
If some countries lead by example, standards may increasingly become normalized
LIDIA MORAWSKA, JOSEPH ALLEN, [...] AND MAOSHENG YAO +40 authors Authors Info & Affiliations
SCIENCE • 28 Mar 2024 • Vol 383, Issue 6690 • pp. 1418-1420

July 6, 2022

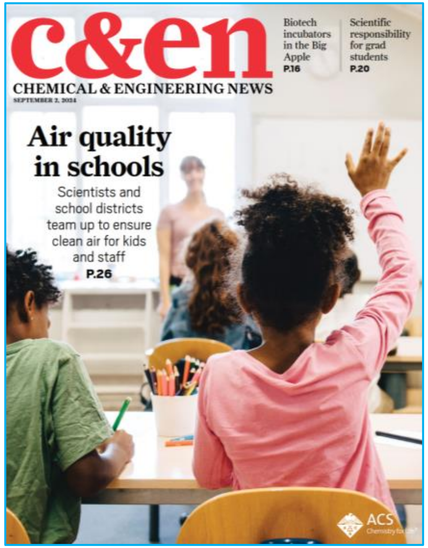


https://www.weforum.org/agenda/2022/07/what-causes-indoor-air-pollution-sources-how-to-reduce/

February 29, 2024

https://prohvacinsights.com/indoor-air-quality-101/

Sept 2, 2024



https://cen.acs.org/analytical-chemistry/Indoor-air-monitoring-goes-school

Air quality index: Four volatiles and their levels of concern

Ozone O_3 < 0.1 ppm
Nitrogen dioxide NO_2 < 0.2 ppm
Sulfur dioxide SO_2 < 0.2 ppm
Carbon monoxide CO <30 ppm

Concentrations of concern:
Brunekreef, Holgate, *Lancet* **2002,** 360, 1233–1242
who.int/ceh/capacity/Outdoor_air_pollution.pdf

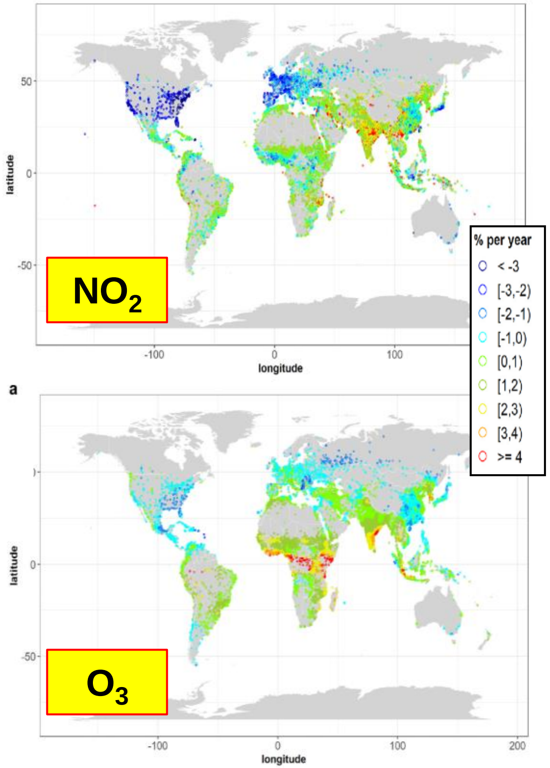
AQI	AQI
I_{low} - I_{high}	Category
0-50	Good
51-100	Moderate
101-150	Unhealthy for Sensitive Groups
151-200	Unhealthy
201-300	Very Unhealthy
301-400	Hazardous
401-500	

Technical Assistance Document for the Reporting of Daily Air Quality – the Air Quality Index (AQI). US EPA Office of Air Quality Planning and Standards. EPA-454/B-09-001, **2009**
Revised Air Quality Standards For Particle Pollution And Updates To The Air Quality Index (AQI). US EPA Office of Air Quality Planning and Standards. **2013**

Reference and Equivalent Methods Used to Measure National Ambient Air Quality Standards (NAAQS) Criteria Air Pollutants – Vol. 1, EPA/600/R-16/139, **2016**

https://www.awarenessdays.com/awareness-days-calendar/national-clean-air-month-2024/

Annual trends in urban areas over 2000–2019



Sicard, P. *et al. Sci. Total Environ.* **858**, 160064 (2023)

Volatiles and volatile biomarkers in exhaled breath

Volatiles in exhaled breath

Categories of 800+ volatiles in exhaled breath:

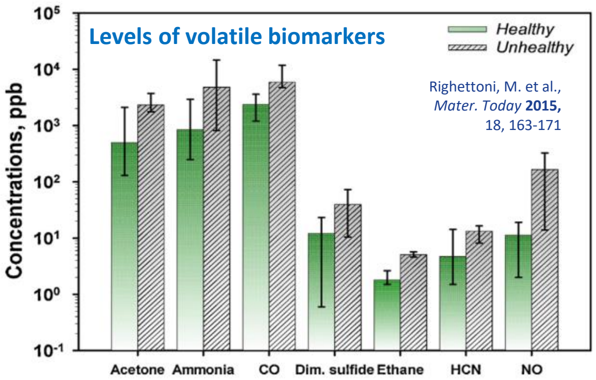
- alkanes,
- alkenes,
- alkynes,
- alcohols,
- aldehydes,
- acids,
- ethers,
- esters,
- ketones,
- nitrogen-, sulfur-, and halogen-containing volatiles,
- benzyl, and phenyl hydrocarbons

de Lacy Costello, et al., J. Breath Res. **2014**, 8, 1–29

Volatile biomarkers of health condition

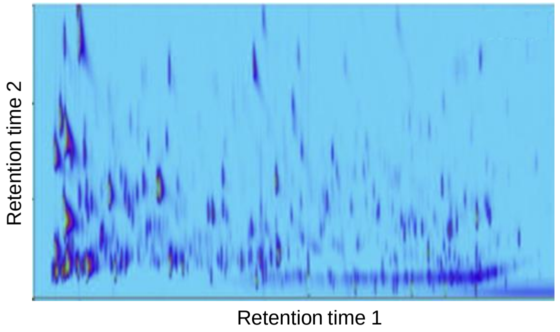
Sample	Disorder/Infection	Volatile compounds
Microorganism-associated disorders		
Urine	Urinary tract infection	Isovaleric acid, alkanes
Intraperitoneal fluid	Aerobic Gram-negative bacteria	Terpenes, ketones
Other disorders		
Human breath	Breast cancer	Alkanes, monomethylated alkanes
Human breath	Lung cancer	Alkanes, monomethylated alkanes
Human breath	Acute asthma	Pentane
Urine	Metabolic disorders	Isovaleric acid
Alveolar air	Hepatic coma	Methyl-mercaptan
Alveolar air	Rheumatoid arthritis	Pentane
Alveolar air	Schizophrenia	Pentane, carbon disulphide
Alveolar air	Ketosis	Acetone

Turner, A. P. F.; Magan, N. *Nat. Rev. Microbiol.* **2004,** 2, 160-166



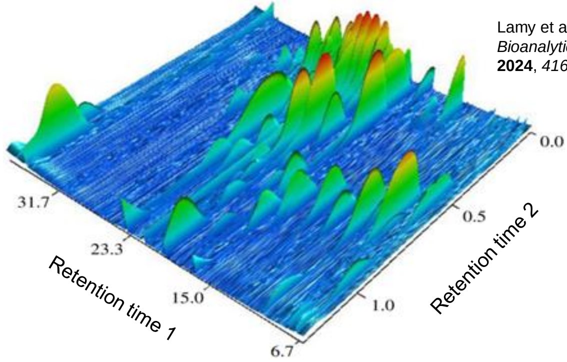
Righettoni, M. et al., *Mater. Today* **2015,** 18, 163-171

Examples of exhaled breath analysis



GCxGC

Wilde et al., *Journal of Chromatography A* **2019,** *1594*, 160-172



GCxGC-TOFMS

Lamy et al., *Analytical and Bioanalytical Chemistry* **2024**, *416*, 4929-4939

GCxGC = two-dimensional gas chromatography
TOFMS = time-of-light mass spectrometry

Examples of standards and guidelines for gas detectors

2022 SEMI | MEMS & SENSORS INDUSTRY GROUP

SEMI MS14-0422 Standard:
Critical parameters of gas sensors for emerging applications

Primary application	Standards and Guidelines	Ref.
Ambient air quality measurements	ASTM WK64899 New Practice for Performance Evaluation of Ambient Air Quality Sensors and Other Sensor-Based Instruments	[1]
Indoor air quality	UL Environment Standard 2905 Environmental Claim Validation Procedure for Indoor Air Quality (IAQ) Sensor Performance	[2]
Toxic and combustible gas and vapor detectors and sensors in indoor / outdoor locations	UL 2075 Standard for Gas and Vapor Detectors and Sensors	[3]
Workplace atmospheres	IEC 62990-1 Workplace atmospheres - Part 1: Gas detectors - Performance requirements of detectors for toxic gases	[4]
Workplace safety	IEC 60079-29-1 Explosive atmospheres - Part 29-1: Gas detectors - Performance requirements of detectors for flammable gases	[5]
Detection of oxygen and toxic levels of gases and vapors	AS/NZS 4641 Electrical equipment for detection of oxygen and other gases and vapours at toxic levels - General requirements and test methods	[6]
Commercial / industrial (non-residential) safety applications	ANSI/ISA 12.13.01-2013, Explosive Atmospheres - Part 29-1: Gas Detectors - Performance Requirements Of Detectors For Flammable Gases	[7]
Toxic gases in commercial / industrial locations	ANSI/ISA-92.00.01-2010 (R2015), Performance Requirements for Toxic Gas Detectors	[8]
Homeland security	ASTM E2885 - 13 Standard Specification for Handheld Point Chemical Vapor Detectors (HPCVD) for Homeland Security Applications	[9]
Marine environments	MSC.1/Circ.1370 Guidelines for the design, construction and testing of fixed Hydrocarbon gas detection systems	[10]
Department of Defense and commercial applications	MIL-STD-810H Department of Defense Test Method Standard	[11]

1. *ASTM WK64899 New Practice for Performance Evaluation of Ambient Air Quality Sensors and Other Sensor-Based Instruments*. ASTM, https://www.astm.org/DATABASE.CART/WORKITEMS/WK64899.htm: 2018.
2. *UL 2905 Environmental Claim Validation Procedure for Indoor Air Quality (IAQ) Sensor Performance*. Underwriters Laboratories, https://standardscatalog.ul.com/ProductDetail.aspx?productId=ULE2905_1_S_20200519: 2020.
3. *UL 2075 Standard for Gas and Vapor Detectors and Sensors*. Underwriters Laboratory, https://standardscatalog.ul.com/ProductDetail.aspx?productId=UL2075: 2013.
4. *IEC 62990-1 Workplace atmospheres - Part 1: Gas detectors - Performance requirements of detectors for toxic gases*. International Electrotechnical Commission, https://www.techstreet.com/standards/iec-62990-1-ed-1-0-b-2019?product_id=2081273: 2019.
5. *IEC 60079-29-1 Explosive atmospheres - Part 29-1: Gas detectors - Performance requirements of detectors for flammable gases CONSOLIDATED EDITION*. International Electrotechnical Commission, https://www.techstreet.com/standards/iec-60079-29-1-ed-2-1-b-2020?product_id=2108773#product: 2020.
6. *AS/NZS 4641 Electrical equipment for detection of oxygen and other gases and vapours at toxic levels - General requirements and test methods*. Standards Australia, https://www.standards.org.au/standards-catalogue/sa-snz/mining/el-023/as-slash-nzs--4641-colon-2018: 2018.
7. *ANSI/ISA 12.13.01-2013, Explosive Atmospheres - Part 29-1: Gas Detectors - Performance Requirements Of Detectors For Flammable Gases*. International Society of Automation, https://webstore.ansi.org/Standards/ISA/ANSIISA1213012013?source=preview: 2013.
8. *ANSI/ISA-92.00.01-2010 (R2015), Performance Requirements for Toxic Gas Detectors*. American National Standards Institute/International Safety Association, https://www.isa.org/products/ansi-isa-92-00-01-2010-r2015-performance-requireme: 2015.
9. *ASTM E2885 - 13 Standard Specification for Handheld Point Chemical Vapor Detectors (HPCVD) for Homeland Security Applications*. American Society for Testing and Materials, https://www.astm.org/Standards/E2885.htm: 2013.
10. *MSC.1/Circ.1370 Guidelines for the design, construction and testing of fixed Hydrocarbon gas detection systems*. International Maritime Organization, https://www.ocimf.org/media/8189/MSC.1-Circ.1370.pdf: 2010.
11. *MIL-STD-810H Department of Defense Test Method Standard, Environmental Engineering Considerations and Laboratory Tests*. US Department of Defense, Washington, DC, USA, https://www.iest.org/Standards-RPs/MIL-STD-810H: 2019.

Every century – solving practical gas-detection challenges

Las Vegas, NV
January 2024

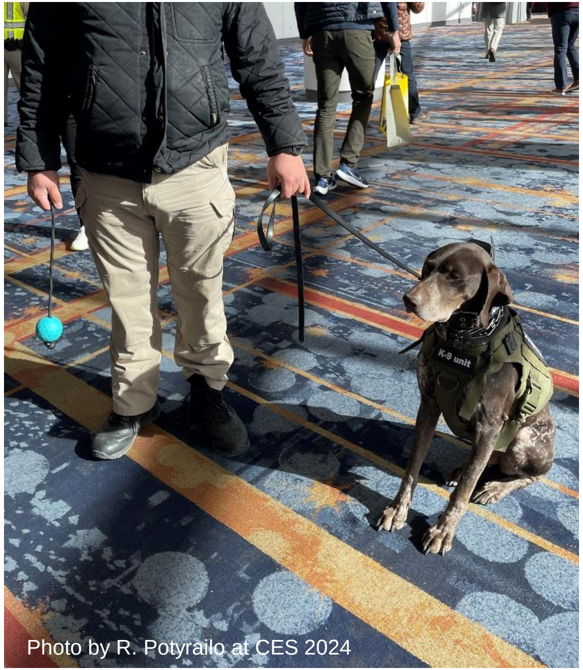


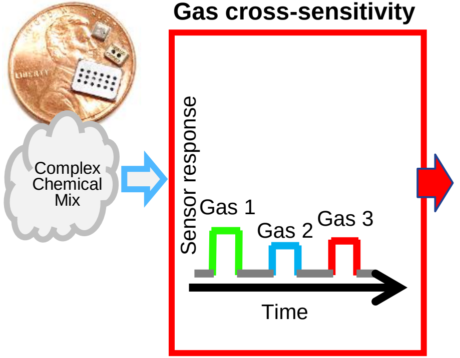
Photo by R. Potyrailo at CES 2024


Photo by R. Potyrailo at CES 2024

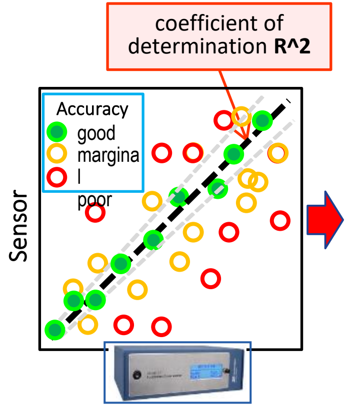
2024:
Security needs and demands drive practical available solutions

Contemporary gas sensors: Gas cross-sensitivity as accepted status quo

Gas cross-sensitivity



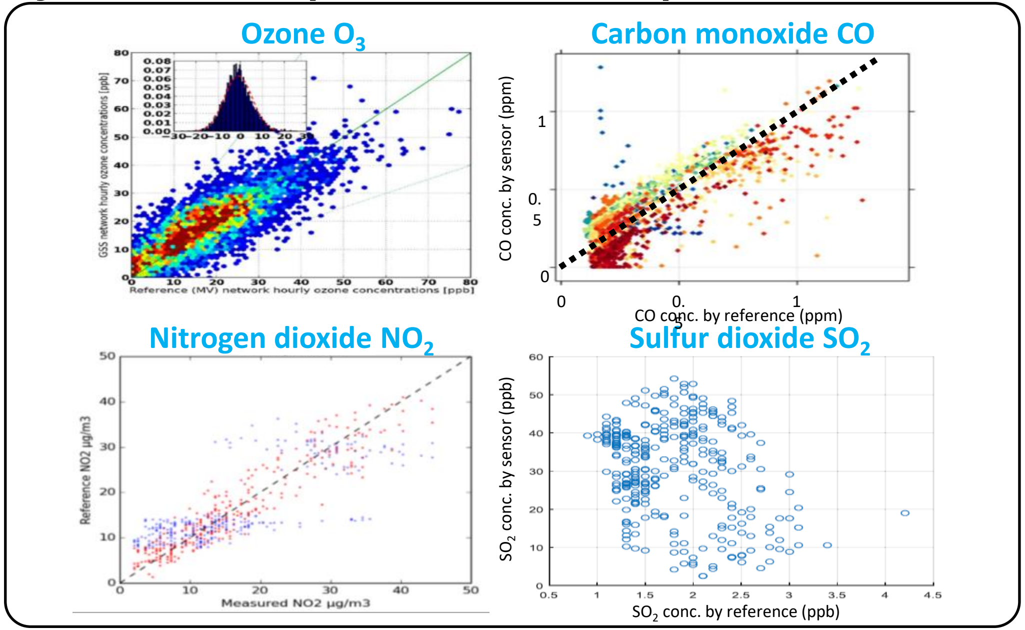
- ✓ Small size
- ✓ Low cost
- ▪ Poor accuracy



Benchmark instrument

A.C. Rai et al., End-user perspective of low-cost sensors for outdoor air pollution monitoring, *Science of the Total Environment* **2017,** *607–608*, 691–705

Bart et al., *Environ. Sci. Technol.* **2014**, *48*, 3970
Hagler et al., *Atmospheric Meas. Tech.* **2016,** 9, 5281
Borrego et al., Atmospheric Environment **2016**, 147, 246
Peterson et al., *Sensors* **2017**, 17, 1653



EPA
It must be stated that no low cost sensors meet the Regulatory Monitoring requirements
-Air Sensor Guidebook, EPA/600/R-14/159, 2014

EPA
Data of poor or unknown quality is less useful than no data since it can lead to wrong decisions
- Environmental Science and Technology, ***2013****, 47, 11369–11377*

nature
The biggest headaches are caused by interfering chemicals
Nature, **2016**, *535*, 29-31

“For the revolution to take off, accuracy must improve”

Contemporary traditional analytical instruments: exquisite performance

Chemiluminescence | **UV fluorescence** | **Laser spectroscopy** | **GC = Gas chromatography** | **MS = Mass spectrometry** | **GC/MS**


Reference and Equivalent Methods Used to Measure National Ambient Air Quality Standards (NAAQS) Criteria Air Pollutants – Vol. 1, EPA/600/R-16/139, **2016**

https://alliedscientificpro.com

draeger.com/en-us_us/Products/X-pid-9000-9500

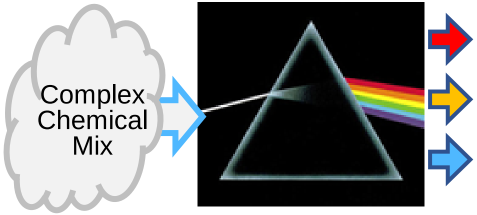
https://908devices.com/products/mx908/

https://www.inficon.com/en/products/chemical-detection-and-utility-monitoring

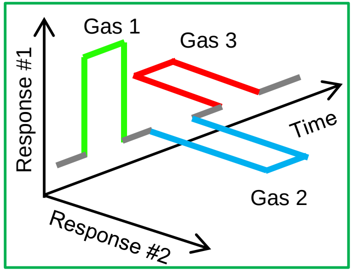
The Nobel Prizes

Chemistry	1952	partition chromatography
Physics	1981	laser spectroscopy
Chemistry	2002	mass spectrometry

Diverse mathematical principles to operate in highly variable unpredictable backgrounds



http://www.yalescientific.org



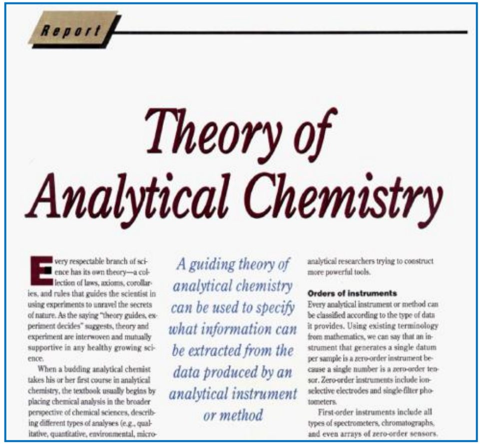
- ✓ Multi-gas detection
- ✓ High accuracy
- ■ Large size
- ■ High cost

Mathematics of analytical instruments: Different orders of measurements

One universe:
Tiny sensors

Another universe:
Much larger SWaP-C traditional exquisite analytical instruments

Booksh, K. S.; Kowalski, B. R. Theory of analytical chemistry, *Anal. Chem.* **1994,** 66, 782A-791A



Report

Theory of Analytical Chemistry

Every respectable branch of science has its own theory—a collection of laws, axioms, corollaries, and rules that guides the scientist in using experiments to unravel the secrets of nature. As the saying "theory guides, experiment decides" suggests, theory and experiment are interwoven and mutually supportive in any healthy growing science.

When a budding analytical chemist takes his or her first course in analytical chemistry, the textbook usually begins by placing chemical analysis in the broader perspective of chemical sciences, describing different types of analyses (e.g., qualitative, quantitative, environmental, micro-

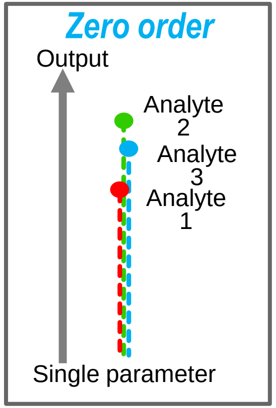
A guiding theory of analytical chemistry can be used to specify what information can be extracted from the data produced by an analytical instrument or method

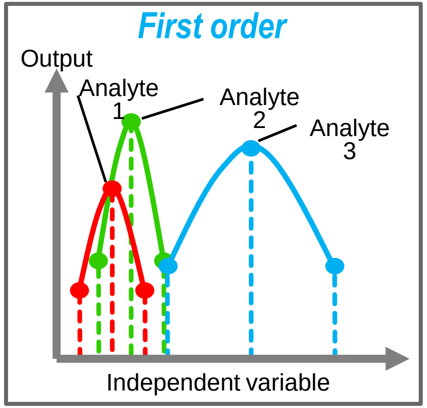
analytical researchers trying to construct more powerful tools.

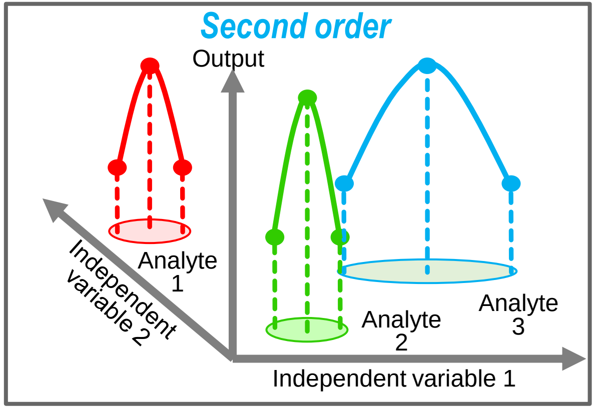
Orders of instruments

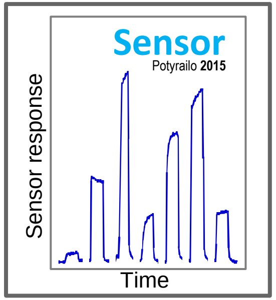
Every analytical instrument or method can be classified according to the type of data it provides. Using existing terminology from mathematics, we can say that an instrument that generates a single datum per sample is a zero-order instrument because a single number is a zero-order tensor. Zero-order instruments include ion-selective electrodes and single-filter photometers.

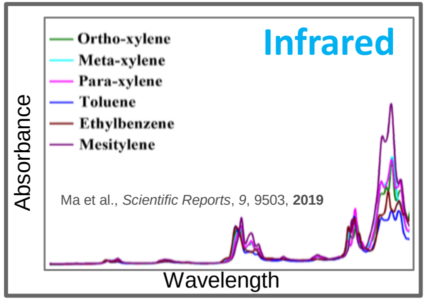
First-order instruments include all types of spectrometers, chromatographs, and even arrays of zero-order sensors.

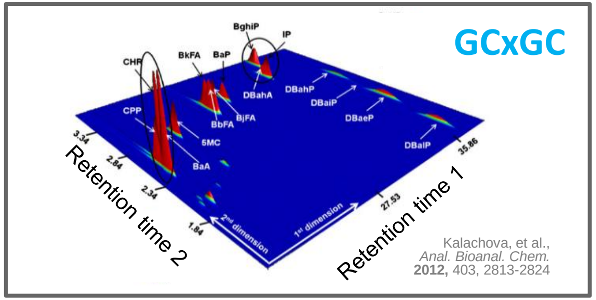










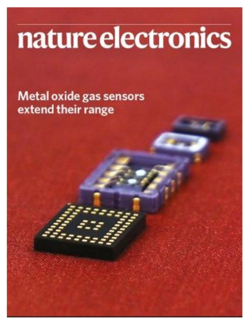


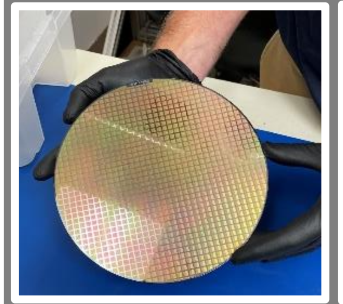
No rejection of interferences

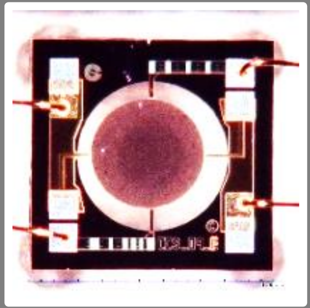
Rejection of known interferences

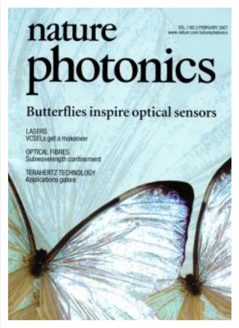
Rejection of unknown interferences

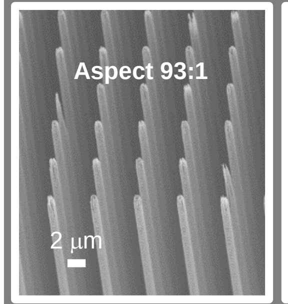
Our roadmap: electromagnetic multivariable gas sensors

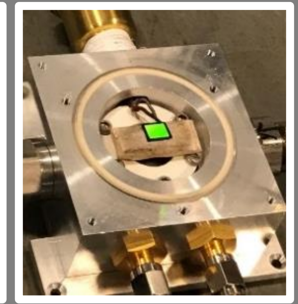








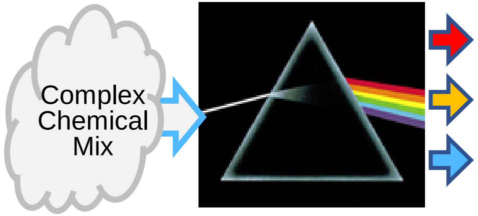




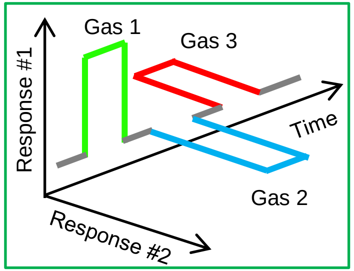
Radio and microwave frequencies

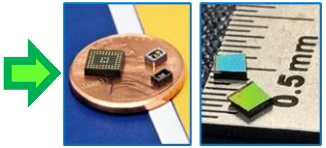
Optical frequencies

Photos by GE Research, R. Potyrailo



http://www.yalescientific.org





www.cdc.gov/niosh/mining/features/GEGasSensor.html

www.genewsroom.com/press-releases/ge-researchers-demonstrate-grain-size-gas-sensor-bloodhound-sensing-capabilities

- ✓Multi-gas detection
- ✓High accuracy
- ✓Small size
- ✓Low cost

Cross-pollination of electronics **+** mathematics **=**
un-anticipated performance boost in ***multivariable*** gas sensors

Tools for data analysis of multivariable sensors:

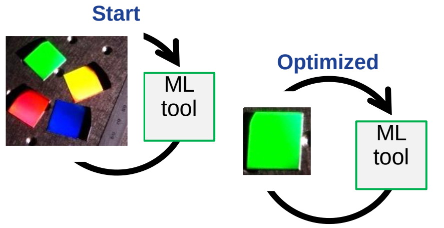
Chemometrics, machine learning (ML), data analytics, multivariate statistics

Data analytics

- Artificial Neural Network (ANN)
- Convolutional Neural Network (CNN)
- Principal component analysis (PCA)
- Discriminant Analysis (DA)
- Hierarchical cluster analysis (HCA)
- Support Vector Machines (SVM)
- Independent Component Analysis (ICA)
- Partial least squares (PLS) regression
- Principal Component Regression (PCR)

Potyrailo *Chem. Rev*. **2016**

ML for sensor system optimization



Potyrailo et al., *Faraday Transactions* **2020**

New tools boost sensor stability, selectivity, sensitivity

Potyrailo, *Chem. Soc. Rev*. **2017**

Potyrailo, et al., IEEE SENSORS, Paper 2381, **2022**

Potyrailo, et al., IEEE SENSORS, Paper 2385, **2022**

Potyrailo, et al., *Appl. Spectrosc.*, **2023**

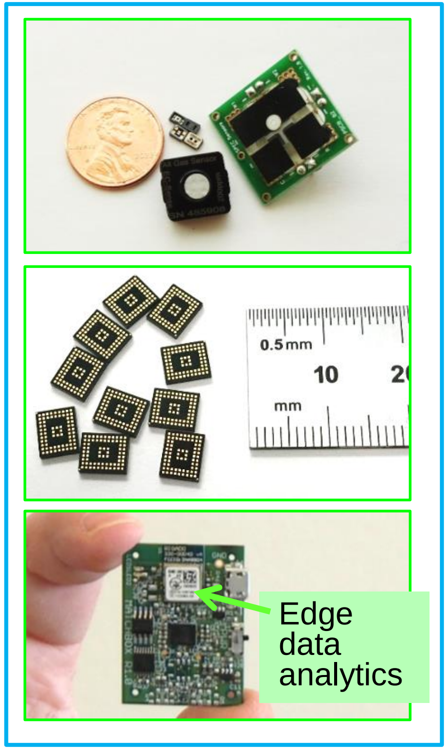
Potyrailo, et al., UPEC 2024, Paper 40, **2024**

Illustrative flow-down requirements: User → system → component

- Maintenance schedule
- Certifications

- Accuracy
- Power
- Calibration
- Communication

- Selectivity
- Sensitivity
- Stability
- Speed

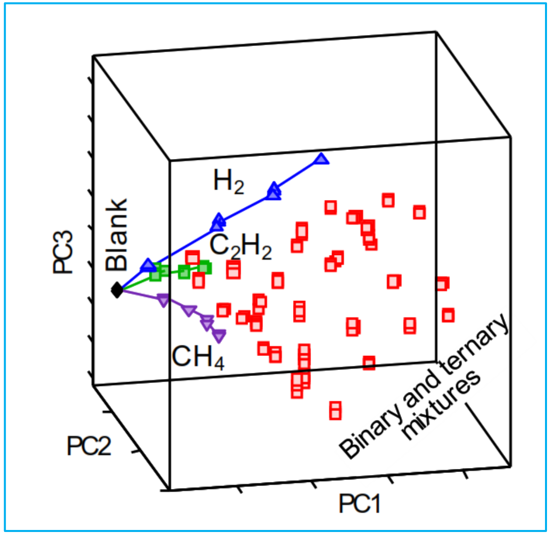


Photos: by R. Potyrailo and by GE team

Illustrative data visualization tools in multi-parameter responses in gas detection

Principal Components Analysis (PCA)

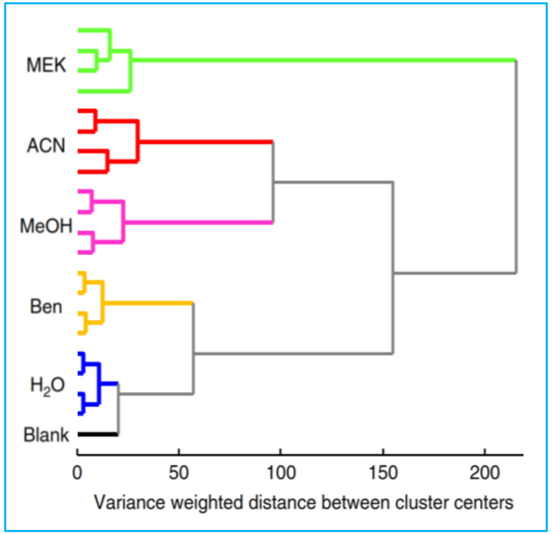
Unsupervised pattern recognition algorithm
Reduces dataset to orthogonal PCs



Potyrailo, et al., *Nat. Electron.* **2020,** 3, 280–289

Hierarchical cluster analysis (HCA)

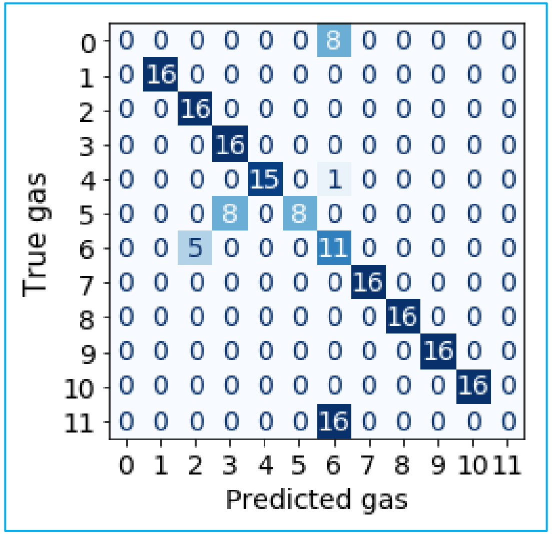
Unsupervised cluster analysis algorithm
Builds clusters by dissimilarities between data



Potyrailo, et al., *Nat. Commun.* **2015,** 6, 7959

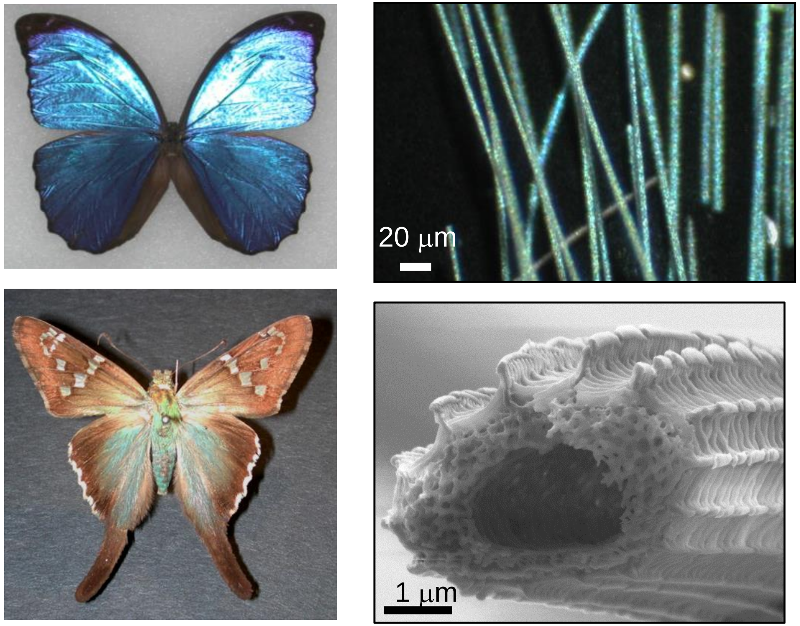
Confusion matrix (a.k.a. error matrix)

Compares Predicted versus True categories
Represents accuracy of classification model

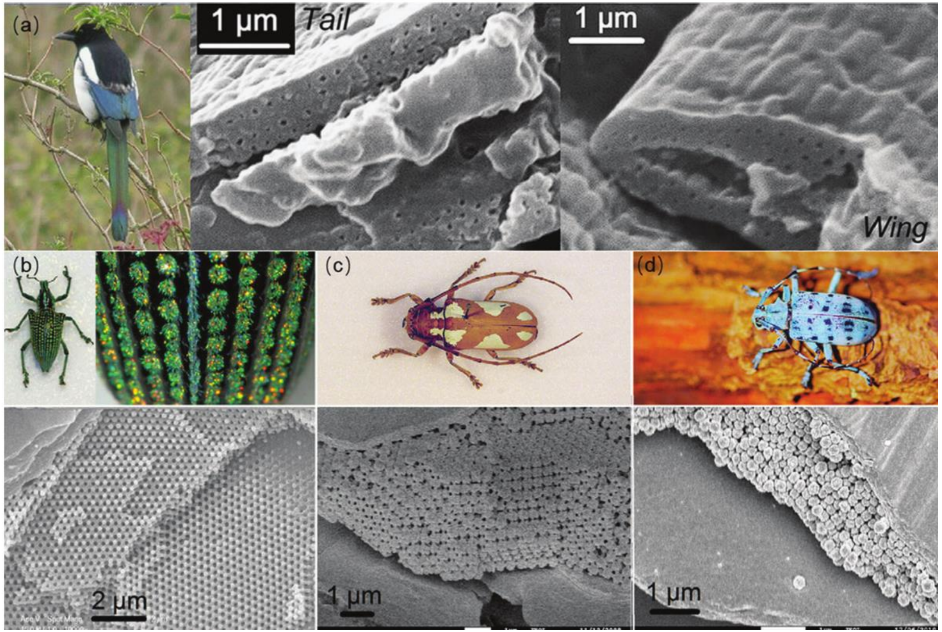


Potyrailo, et al., *2022 CBD S&T Conf.,* **2022**, 159

Examples of natural photonic crystals



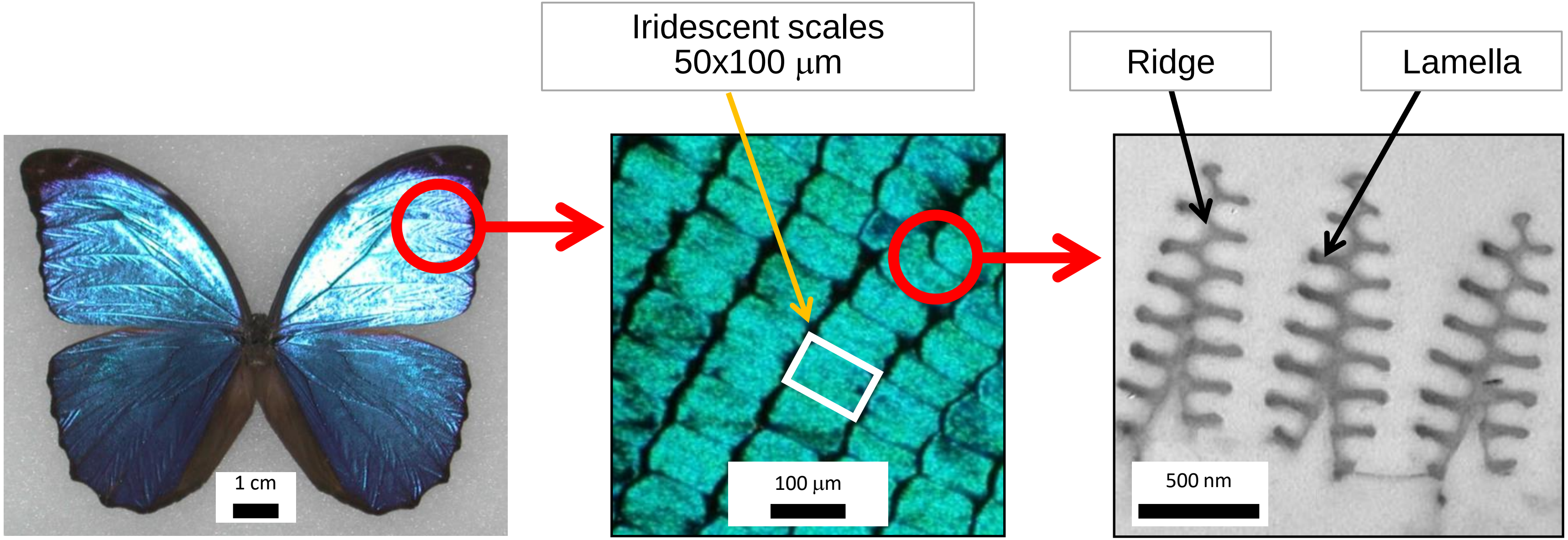
J. Opt. **2018,** 20, 024006



Adv. Mater. Technol. **2024**, 2400865

Bright iridescence is produced by diverse photonic effects

Natural photonic nanostructures as unconventional interfaces for multi-gas sensing ?

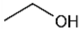


Unique open-to-air photonic nanostructured interface

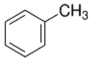
Structural color in nature: from understanding to functional applications

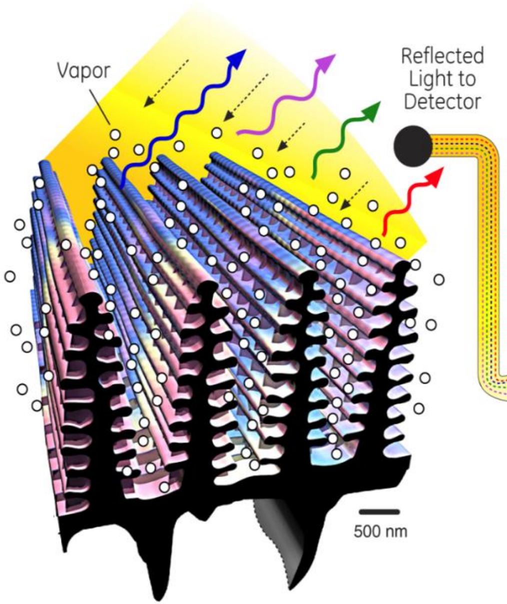
Operation principle of multivariable sensors utilizing natural *Morpho* butterfly scales

Ethanol



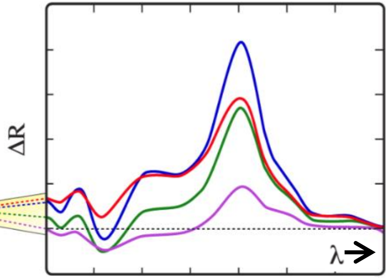
Toluene





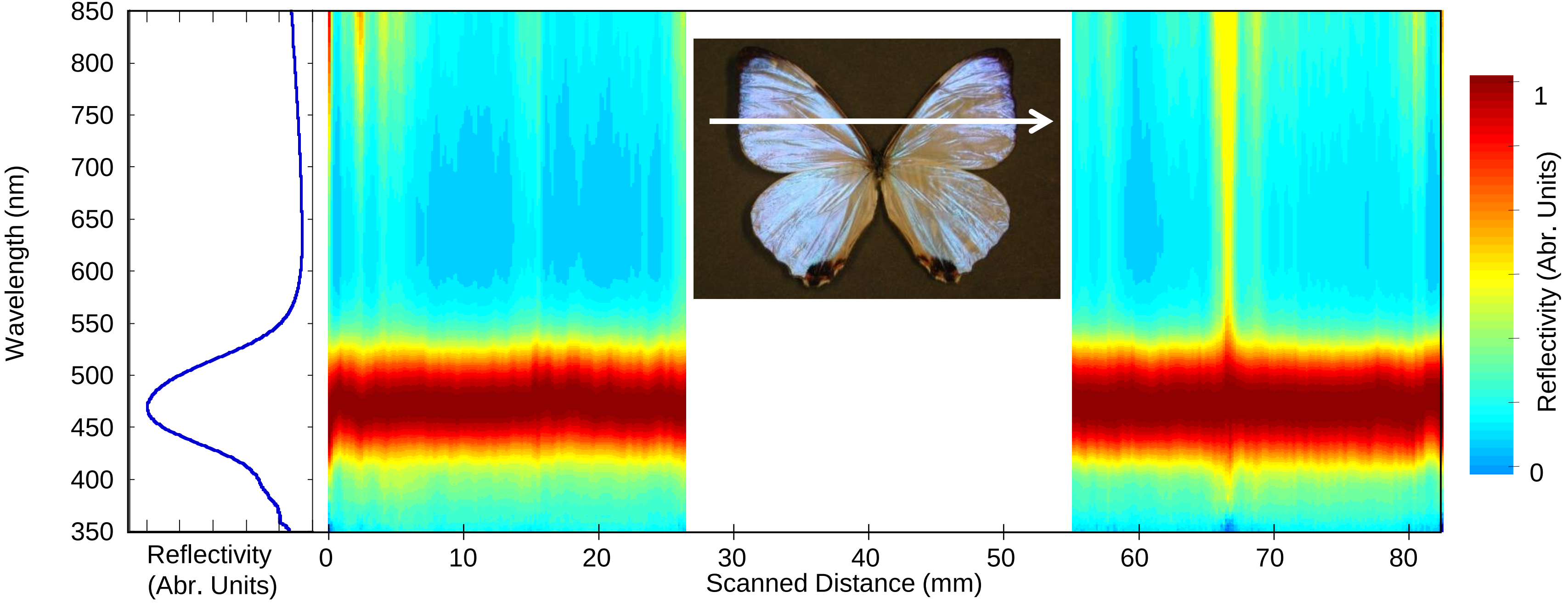
$$\Delta R(\lambda) = R(\lambda)/R_0(\lambda)$$

$R(\lambda)$ spectrum upon vapor exposure
$R_0(\lambda)$ spectrum in clean carrier gas



Research curiosity brings a potential for useful performance

Stability of the reflectivity pattern of *Morpho* scales

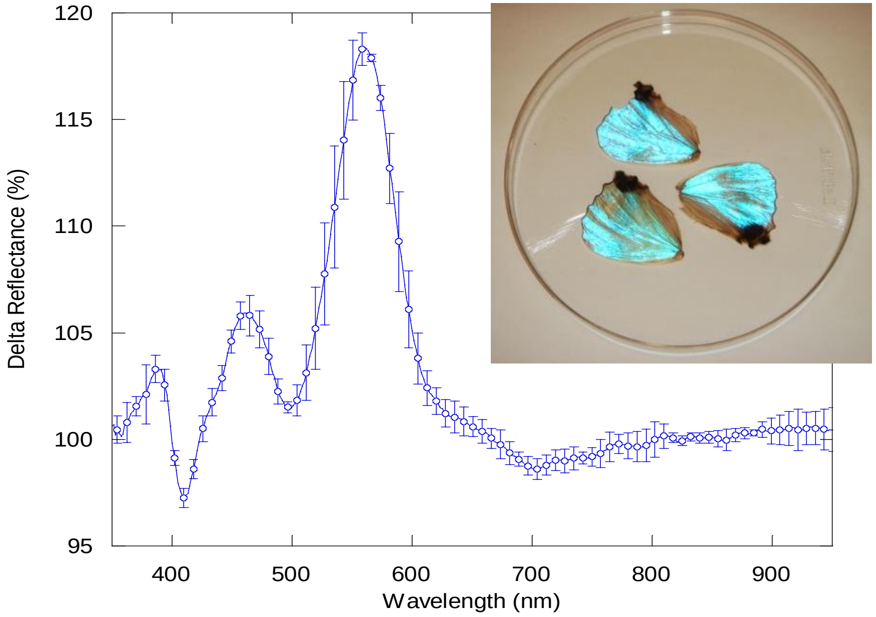


Spatially-resolved (100-um step size) reflectivity of scales of intact butterfly

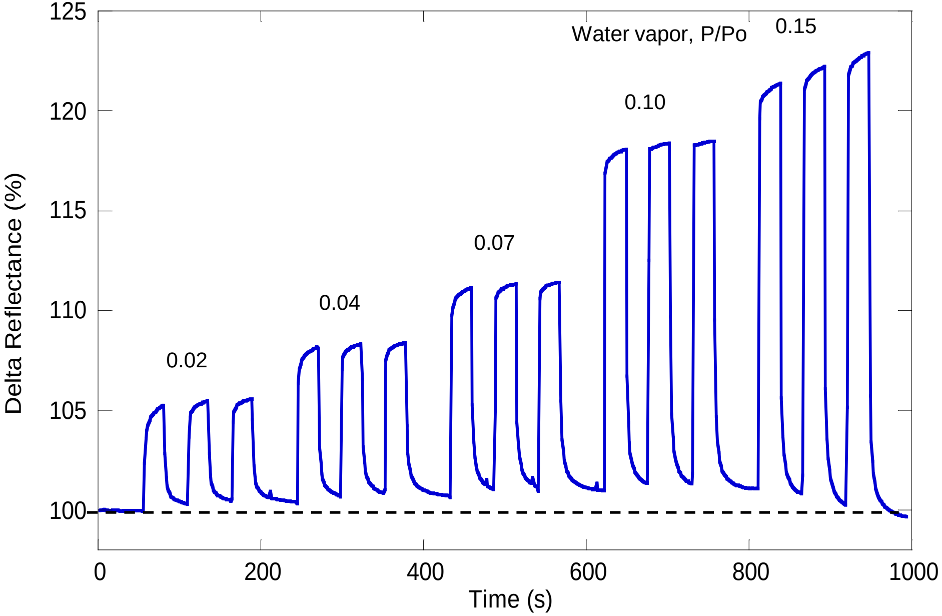
Potyrailo et al., *Nature Photonics*, **2012**

Reproducibility of spectral vapor responses of *Morpho* scales

Reproducibility of ΔR(λ) spectra from different samples (*n* = 3)



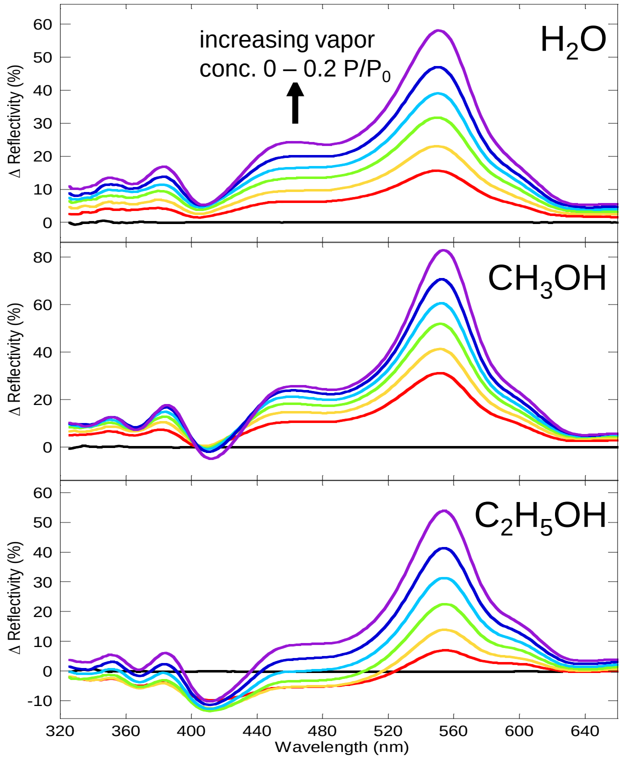
Reproducibility of dynamics and magnitude of response

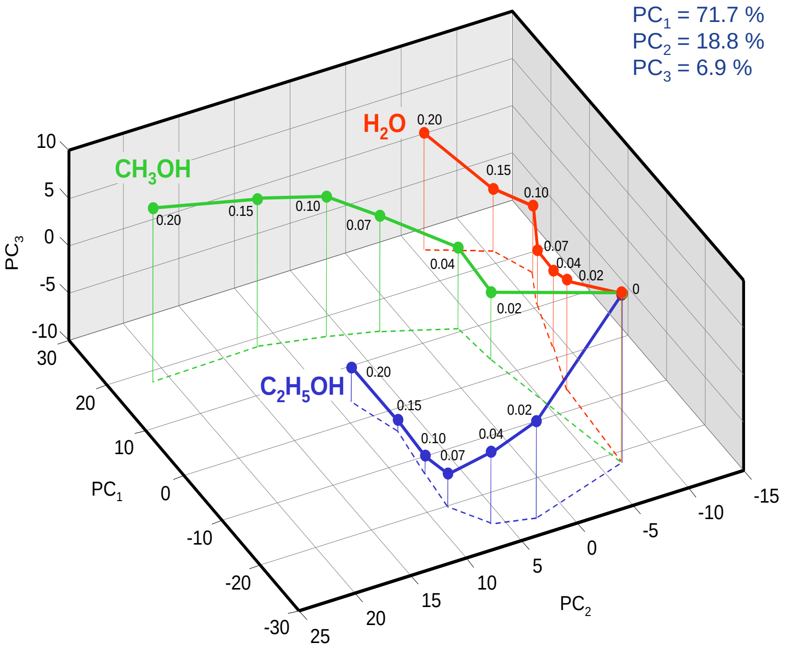


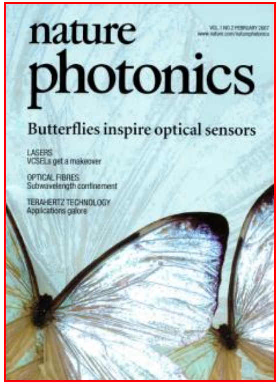
P = vapor partial pressure
P_0 = saturated vapor pressure

Potyrailo et al., *Nature Photonics*, **2012**

Unexpected differentiation of closely related vapors: water, methanol, ethanol



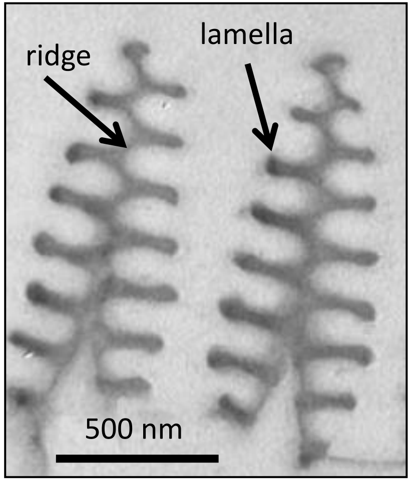


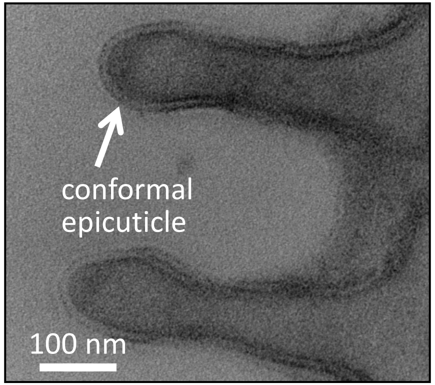


Potyrailo et al., *Nature Photonics* **2007**

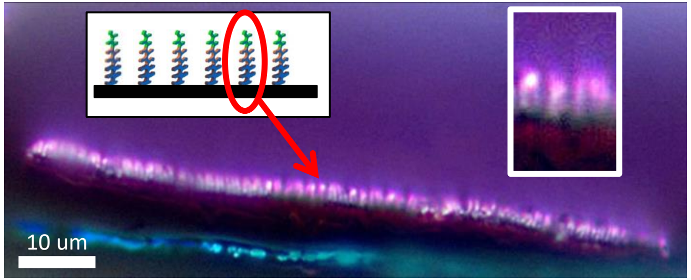
Multivariate spectral analysis reveals extraordinary selectivity of optical response to diverse vapors

Origin of high vapor-response selectivity: polarity gradient of ridges of *Morpho* scales

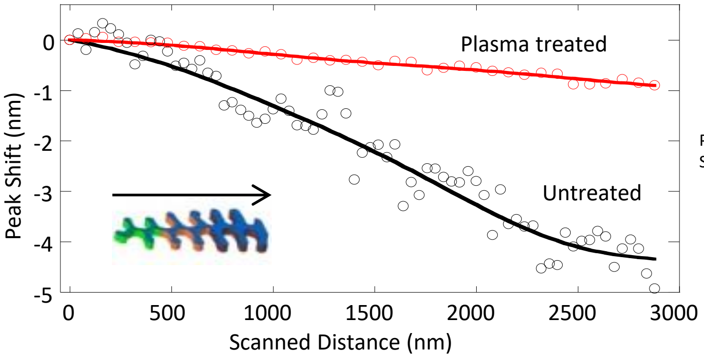




Cross-section of fluorophore-stained ridge structure



Fluorescence peak shift



Plasma treatment = 30 s
Scan step size = 40 nm

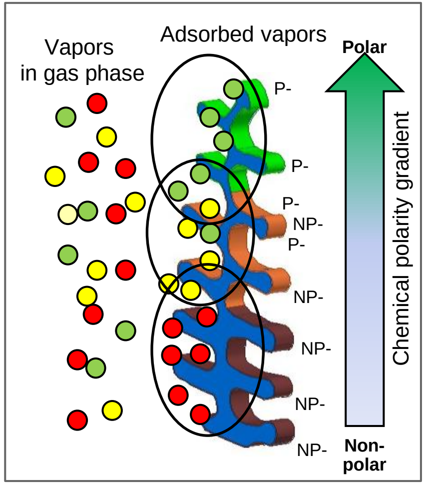
Tops of ridges are more polar than their bottoms as determined by staining with polarity-sensitive dye

Proc. Natl. Acad. Sci. U.S.A. **2013,** 110, 15567–15572

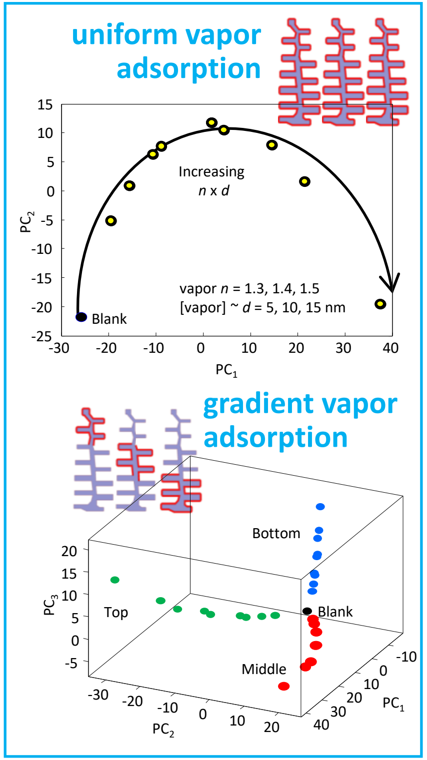
Understanding design rules for bio-inspired photonic sensors: toward multi-gas sensing with fabricated photonic nanostructures

Modelling results

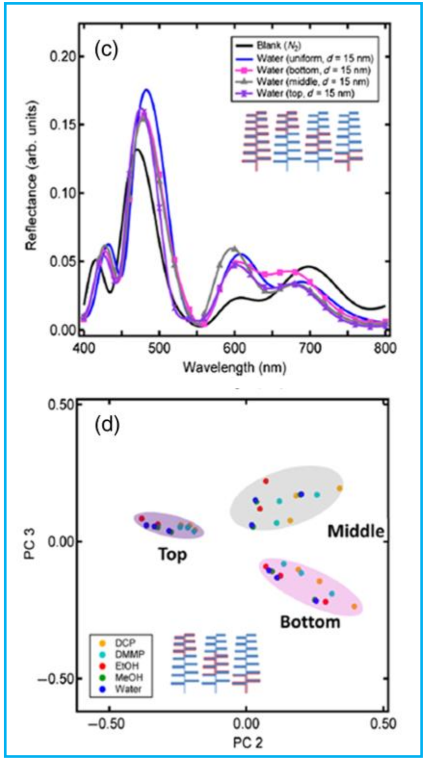
Gradient of surface polarity



Proc. Natl. Acad. Sci. U.S.A. **2013,** 110, 15567–15572

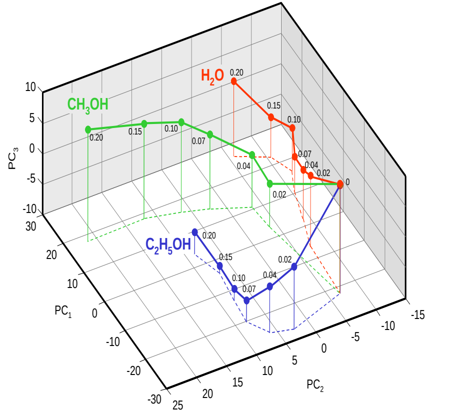


Proc. Natl. Acad. Sci. U.S.A. **2013,** 110, 15567–15572



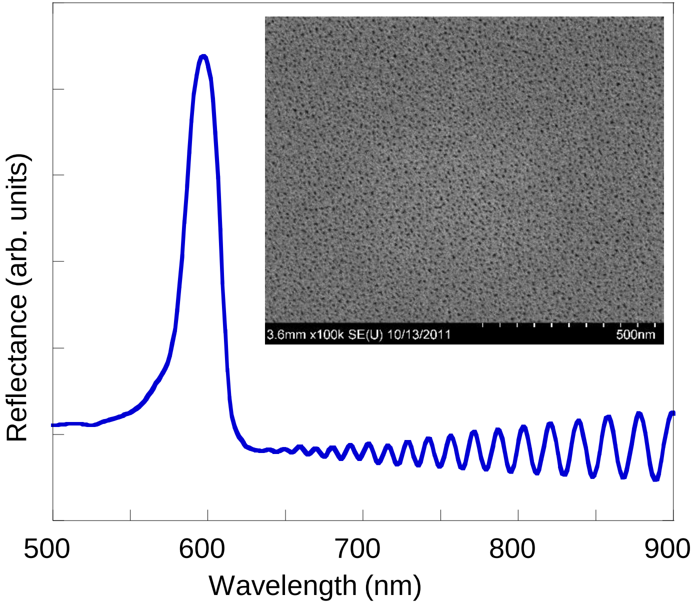
ACS Omega **2017,** 2, 83018307
Journal of Optical Microsystems **2024**, 4, 020902

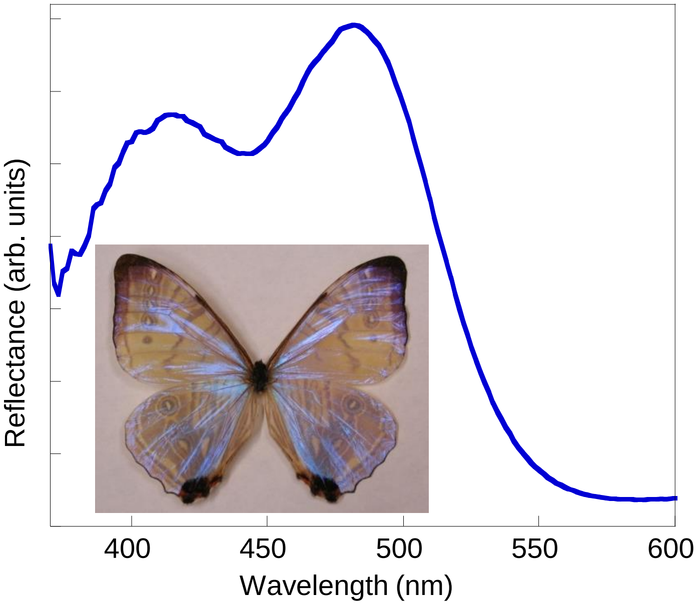
Experimental results



Nat. Photonics **2007,** 1, 123-128

Comparison of *Morpho* scales response with “benchmark” porous Si vapor-sensing material

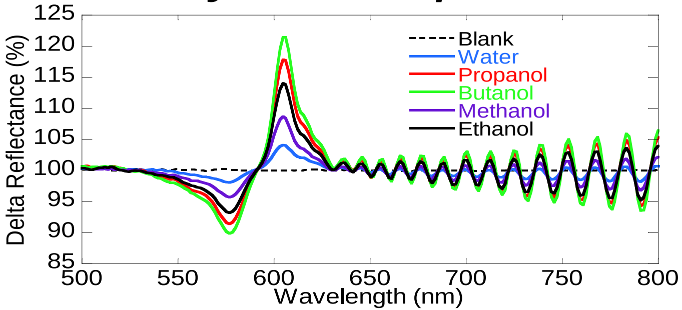


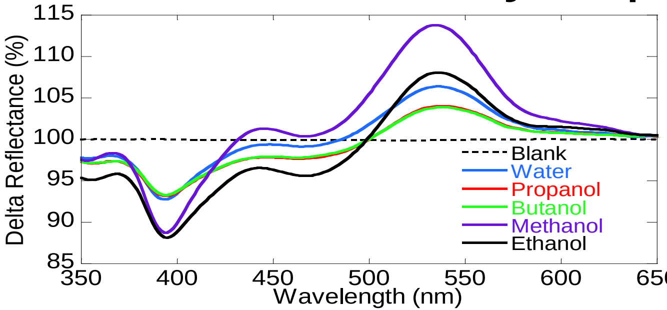


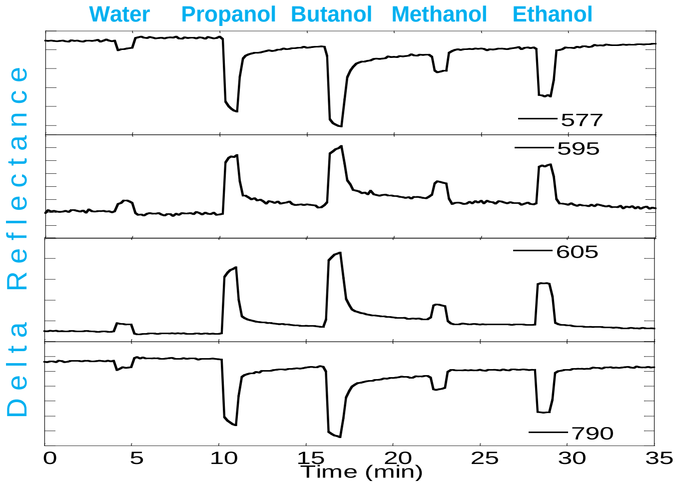
Porous silicon is an ideal control with excellent vapour-sensing properties and demonstrated possibilities for surface functionalization

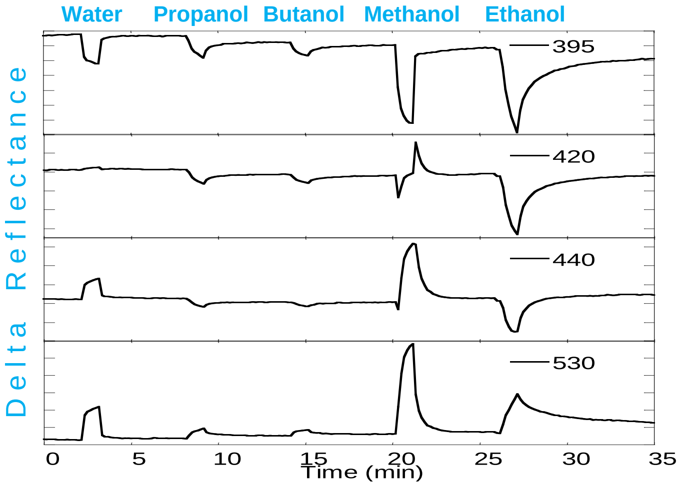
Potyrailo et al., *Proc. Natl. Acad. Sci. U.S.A.* **2013**

Vapor selectivity of *Morpho* scales vs. no-selectivity of porous Si





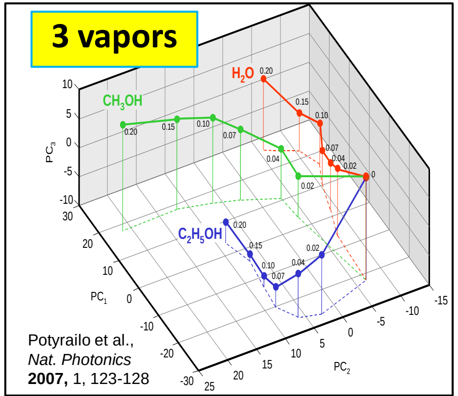




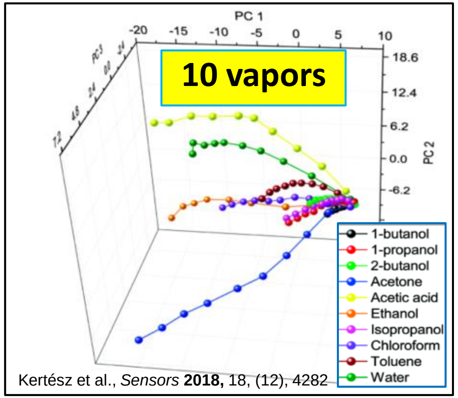
Comparison parameters: (1) relative intensities; (2) directions of responses; (3) dynamics of responses

Potyrailo et al., *Proc. Natl. Acad. Sci. U.S.A.* **2013**

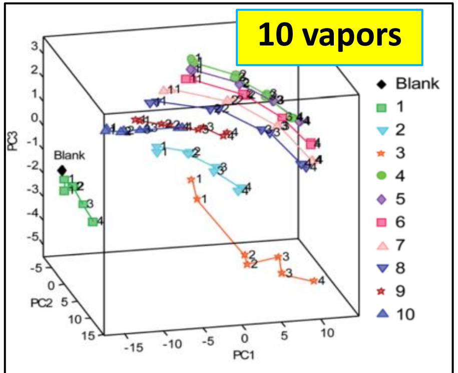
Up to 5-D dispersion with individual natural photonic nanostructures



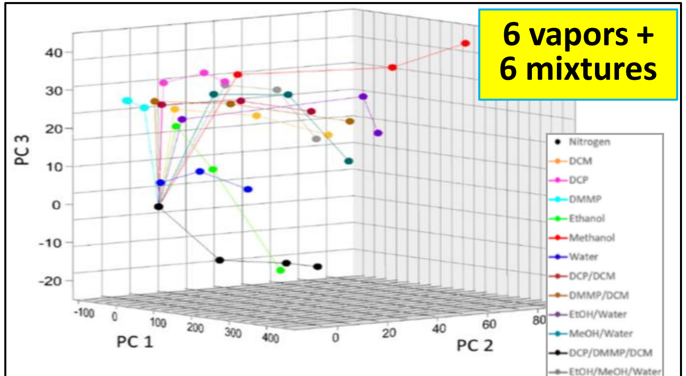
Potyrailo et al., *Nat. Photonics* **2007,** 1, 123-128



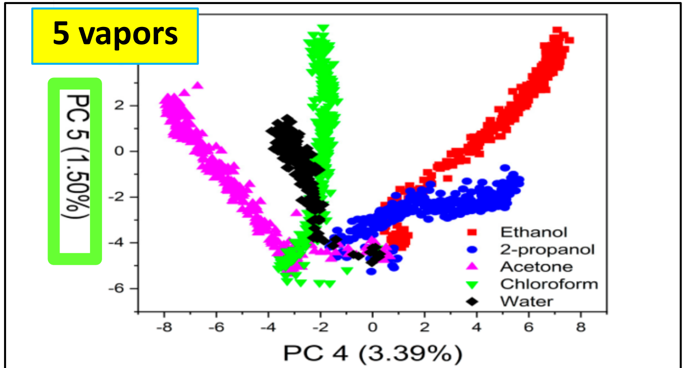
Kertész et al., *Sensors* **2018,** 18, (12), 4282



Potyrailo et al, *Faraday Discuss.* **2020,** 223, 161-182



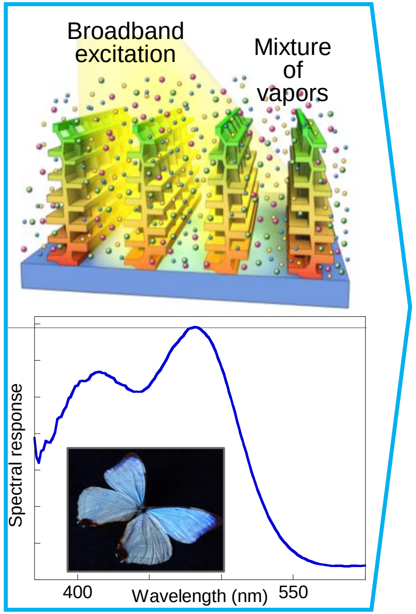
Kittle et al., *Sensors* **2020,** 20, (1), 157

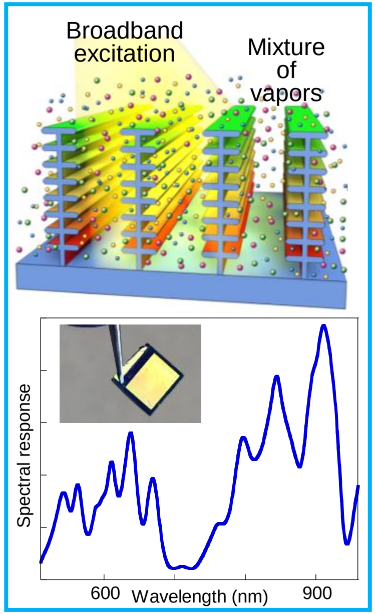


Piszter et al., *Sensors* **2020,** 20, (11), 3258

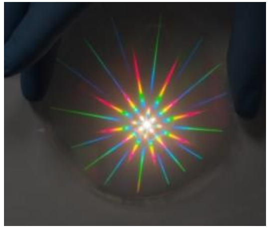
High dispersion allows differentiation of analytes in complex backgrounds

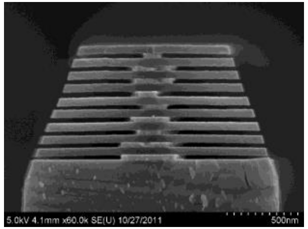
From fundamental science to new insights in multi-gas nanostructured photonic sensors



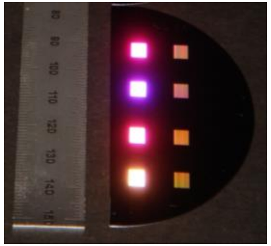


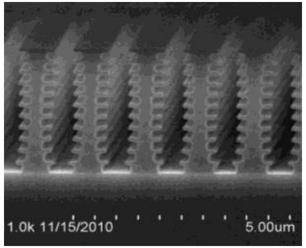
Conventional lithography





E-beam lithography

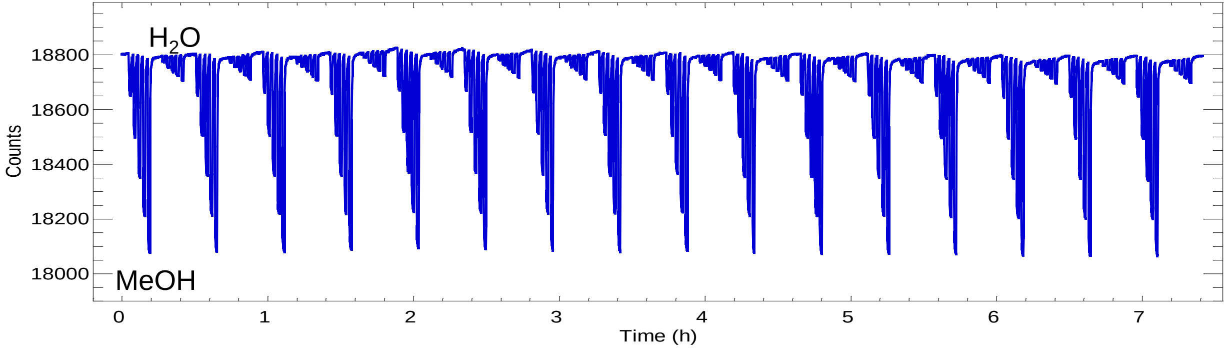




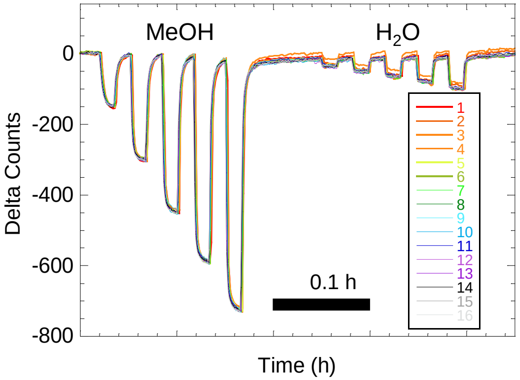
Potyrailo et al. *Nature Communications* **2015**

Design rules for multi-gas differentiation control:
- Spatial orientation of surface functionalization
- Chemistry of surface functionalization
- Extinction and scattering of nanostructure

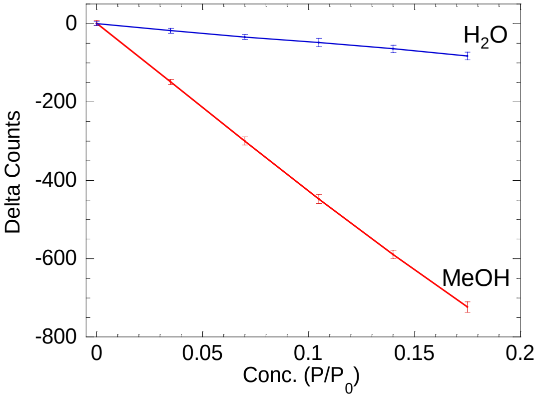
Response stability of nanostructures: 160 cycles of methanol (MeOH) and water (H2O) vapors



Response reproducibility
80 cycles MeOH, 80 cycles H_2O

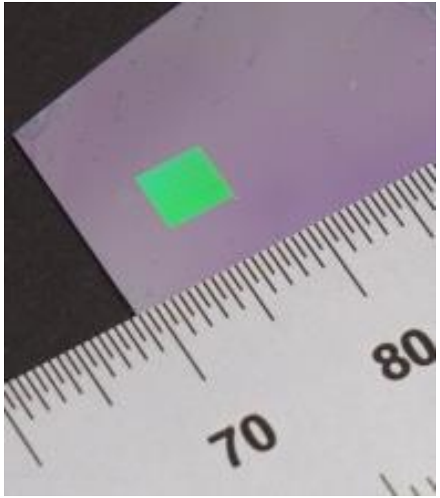


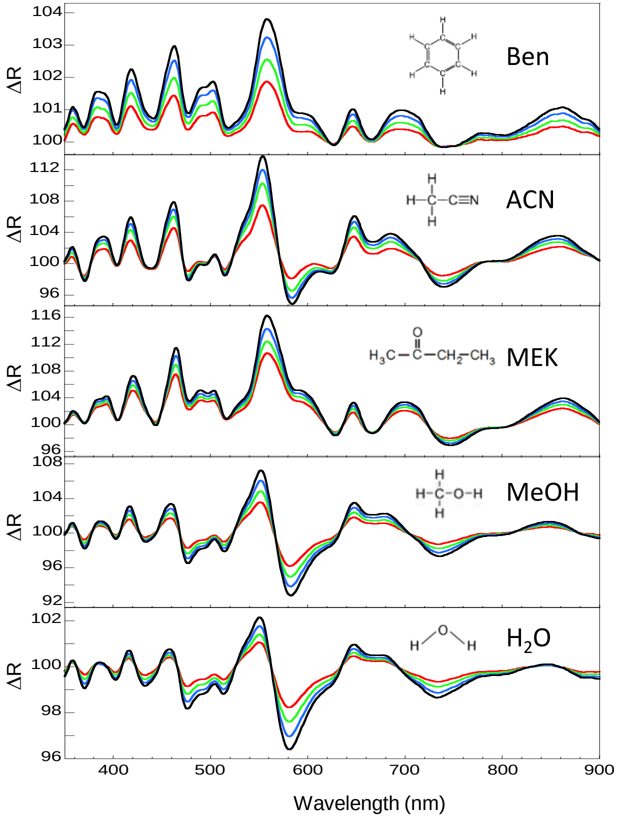
Calibration curves
for MeOH and H_2O



Concentrations of vapors: 0.035, 0.07, 0.105, 0.14, and 0.175 P/P0

Exposures to vapors: differential reflectance spectra





Ben = benzene
ACN = acetonitrile
MEK = methyl ethyl ketone
MeOH = methanol
H2O = water

Concentrations of vapors:
0.05, 0.07, 0.09, 0.11 P/P_0

LOD = limit of detection

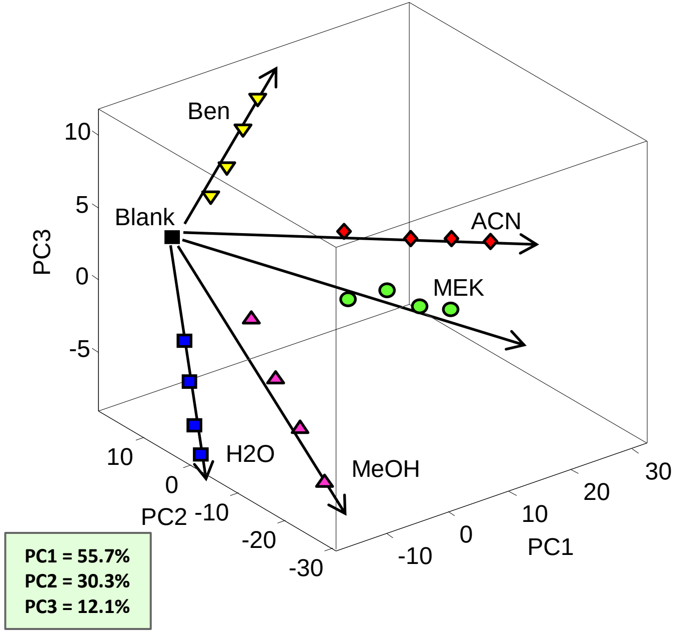
Exemplary vapours	Extrapolated LOD (ppm)
Benzene	45
Acetonitrile	9
Methyl ethyl ketone	7
Methanol	13
Water	8
Ethanol	10
Propanol	3

Potyrailo et al.
Nature Communications **2015**

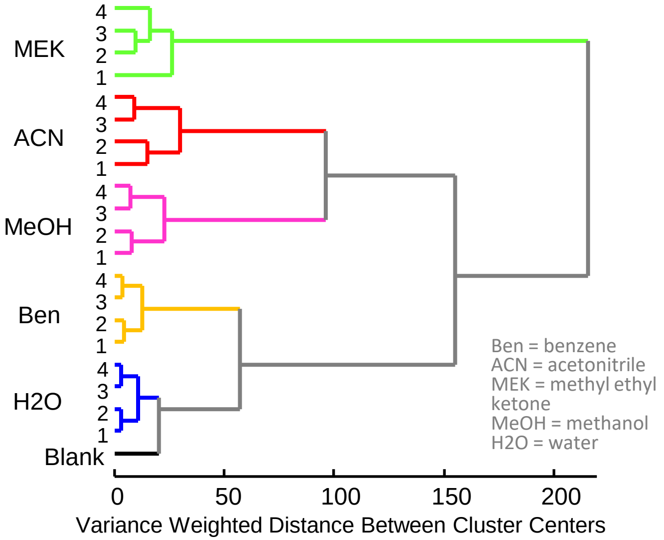
Unique spectral responses to different vapors
reveal diversity of optical interactions probed by individual sensor

Differentiation of vapors

Principal components analysis:
high data dimensionality
on exposure to only several vapors

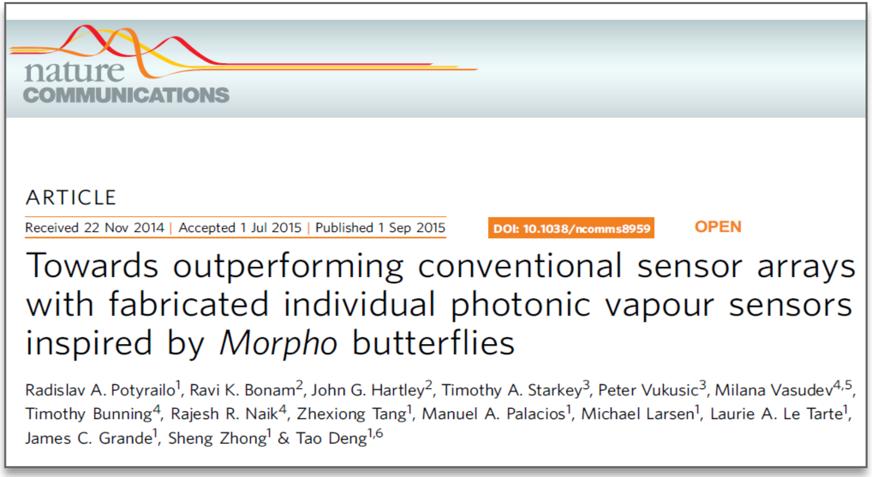


Hierarchical cluster analysis:
classification of vapors
based on raw ΔR spectra



PCA and HCA independently showed clustering based on nature of diverse vapors measured by single multivariable sensor

Single multivariable sensor outperforms sensor arrays



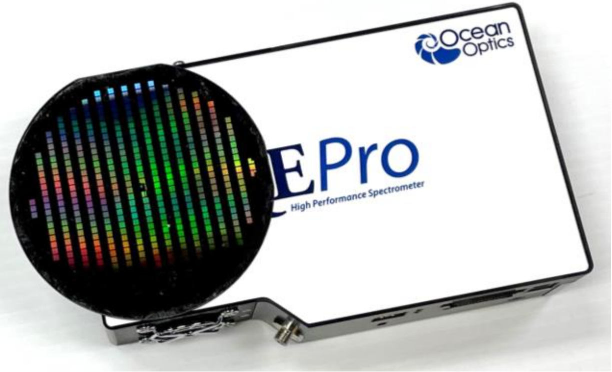
nature COMMUNICATIONS

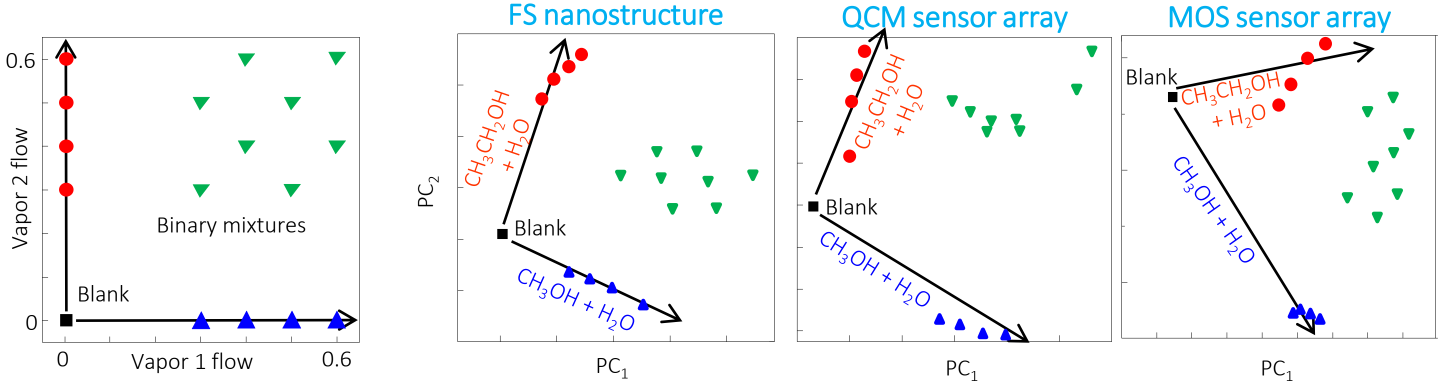
ARTICLE

Received 22 Nov 2014 | Accepted 1 Jul 2015 | Published 1 Sep 2015 DOI: 10.1038/ncomms8959 OPEN

Towards outperforming conventional sensor arrays with fabricated individual photonic vapour sensors inspired by *Morpho* butterflies

Radislav A. Potyrailo[1], Ravi K. Bonam[2], John G. Hartley[2], Timothy A. Starkey[3], Peter Vukusic[3], Milana Vasudev[4,5], Timothy Bunning[4], Rajesh R. Naik[4], Zhexiong Tang[1], Manuel A. Palacios[1], Michael Larsen[1], Laurie A. Le Tarte[1], James C. Grande[1], Sheng Zhong[1] & Tao Deng[1,6]





FS = nonafluorohexyl-trimethoxysilane

QCM = quartz crystal microbalance

MOS = metal oxide semiconductor

Multi-gas sensing:
Dispersion of a dosimeter array vs a multivariable sensor

High dispersion
of a 36-sensor array:

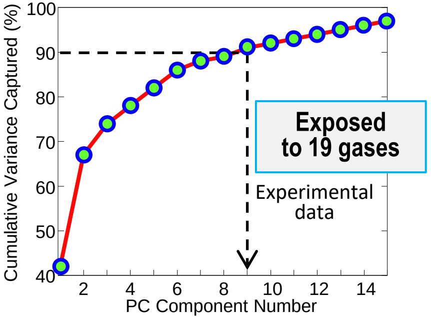
9 dimensions
capture 90% of total variance

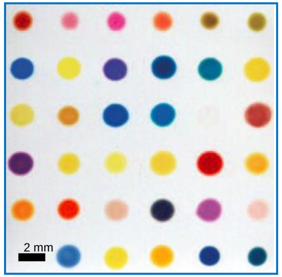
Potyrailo et al. *Chem. Rev.* **2016**

High dispersion
of single multivariable sensor:

11 dimensions
capture 90% of total variance

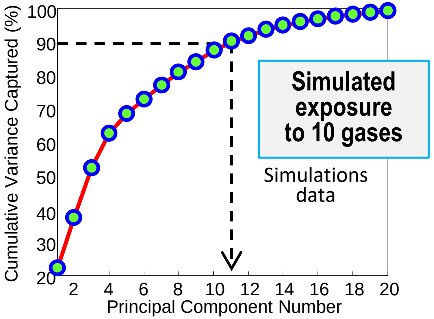
Conventional 36-dosimeter array

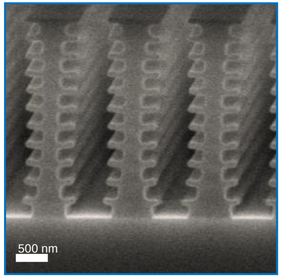




Suslick et al. *Nat. Chem.* **2009**

Individual bio-inspired sensor



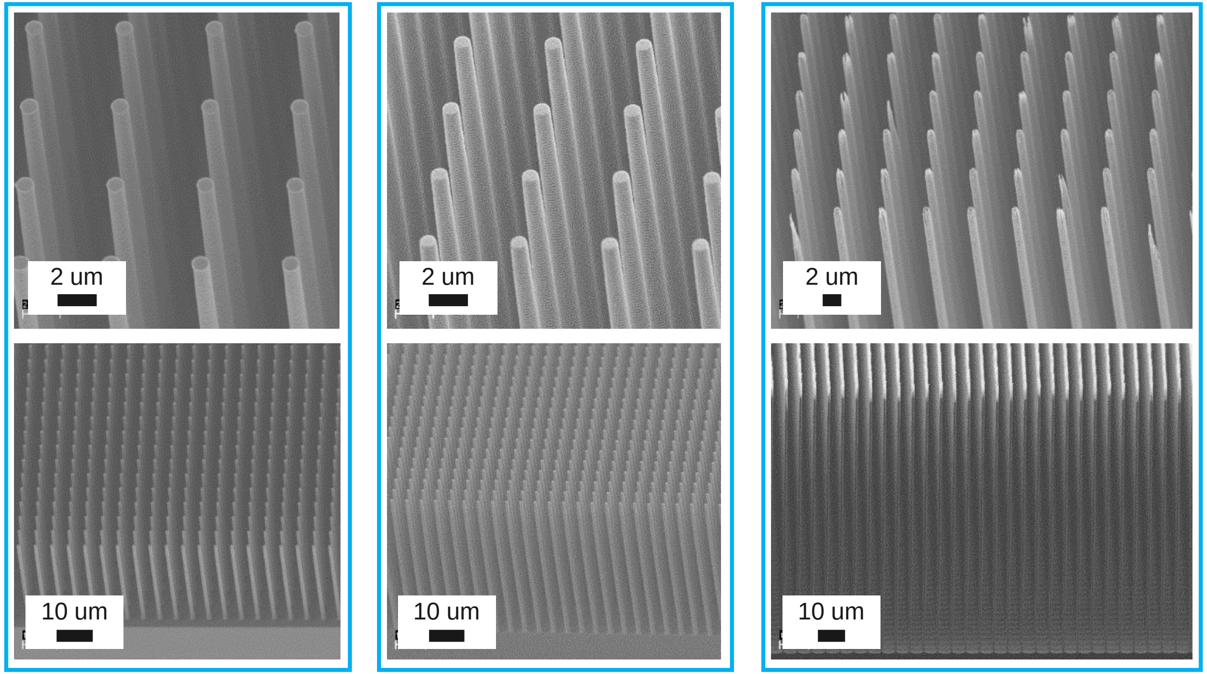


Potyrailo et al. *Nature Comm.* **2015**

New perspective for sensing:
Selectivity within a single nanostructured unit, rather than from an array of colorimetric sensors

Our nanostructured sensing materials w/ exquisite light control

Aspect ratio 43:1 | **Aspect ratio 63:1** | **Aspect ratio 93:1**



Potyrailo, R. A. *Reporting Interfaces: Unconventional Excitation of Interfaces Enables Exquisite Gas Sensing Toward Our Sustainable Future*. (AVS 69th International Symposium & Exhibition, Portland, OR, Nov 5 - 10, Paper 76397, **2023**)

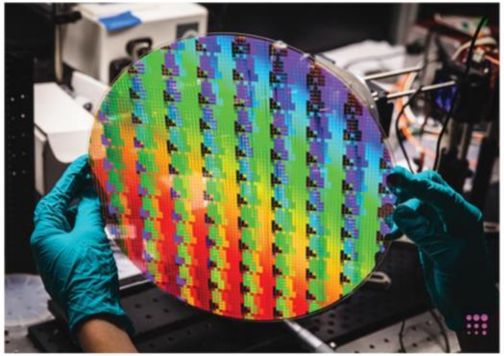
Emerging manufacturing tools

PHOTONICS MEDIA photonics.com

Metalenses Scale Up to Target the Market for Small Optics

As high-volume manufacturing helps metalenses make their debut in consumer electronics this year, the prospects for the technology's growth are anything but flat.

JAMES SCHLETT, CONTRIBUTING EDITOR



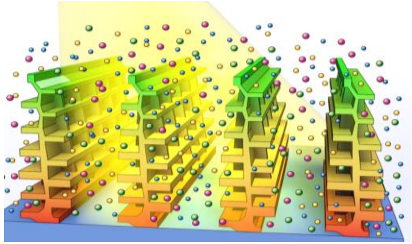
https://www.photonics.com/Articles/Metalenses_Scale_Up_to_Target_the_Market_for/a68722

March 2023

New opportunities for multi-gas sensing using nanostructures with extremely high aspect ratio

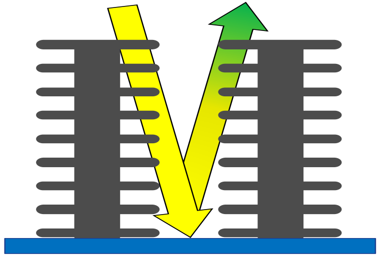
Advancing design rules of nanostructures: high temperature gas-sensing applications

Multi-gas control at room temperature



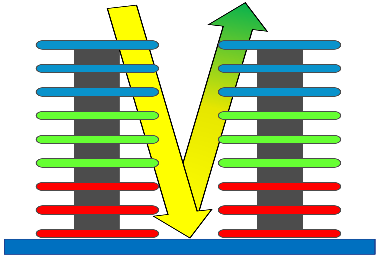
- Polymeric nanostructure
- Absorption and adsorption of vapors

Multi-gas control at high temperature

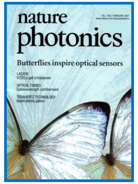


- Inorganic nanostructure
- Catalytic reactions of gases

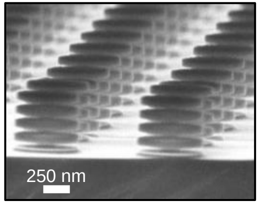
Interference rejection control

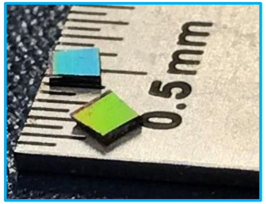


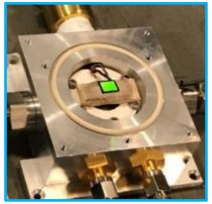
- Multi-material inorganic nanostructure
- Catalytic reactions of gases



Potyrailo et al. *Nature Photonics* **2007**
Potyrailo *Chem. Soc. Rev.* **2017**



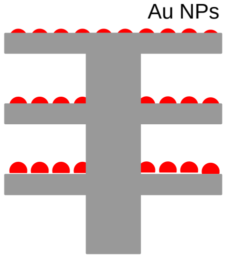


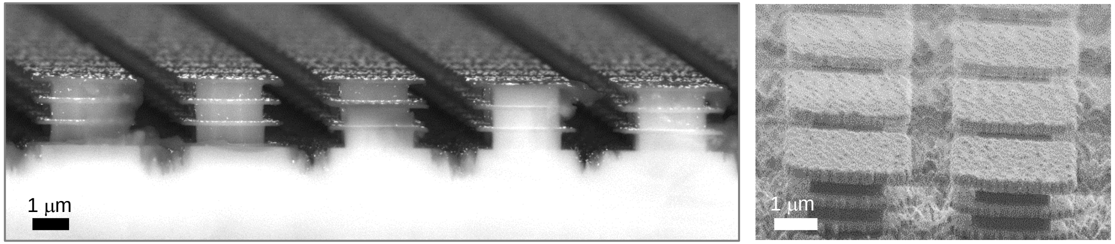


Potyrailo, et al., *J. Opt.* **2018**
Potyrailo, et al., *Appl. Spectrosc.* **2023**

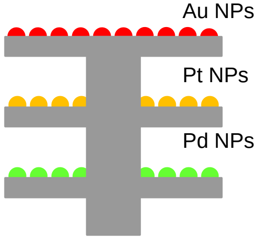
Advancing design rules of nanostructures: high temperature gas-sensing applications

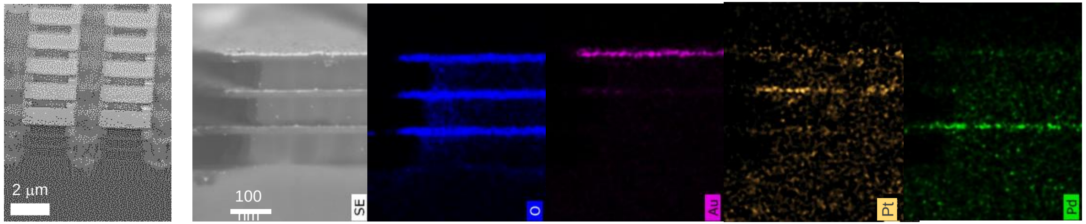
Nanostructure with Au nanoparticles





Nanostructure with Pd, Pt, and Au nanoparticles





Potyrailo, *et al. From Natural to Fabricated Gas Sensing Photonic Nanostructures: Unexpected Discoveries and Societal Impact*. (AVS 69th International Symposium & Exhibition, Portland, OR, Nov 5 - 10, Paper 78421, **2023**)

Analysis by Andrei Kolmakov, NIST

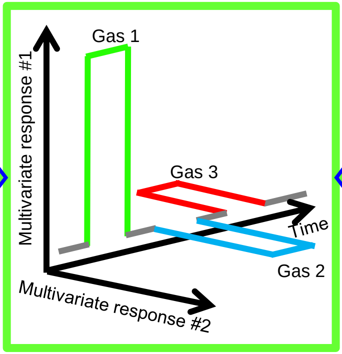
Design rules for multi-gas differentiation control at high temperatures (300C)

- Diversity of catalytic reactivity of nanoparticles (type of noble metal, particle size)
- Spatial distribution of catalytically diverse nanoparticles
- Spectral discrimination of catalytic reactions in different regions of 3D nanostructure

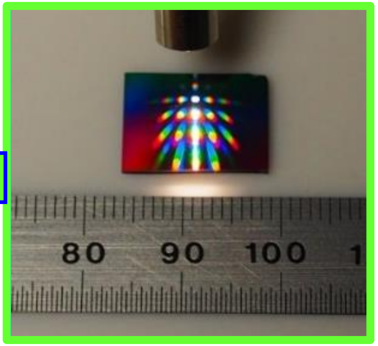
Need for real-time monitoring of H_2 and CO gases in solid oxide fuel cell (SOFC) applications

Status quo:
Mature traditional detector concepts

Performance need:
Compact system for multi-gas discrimination



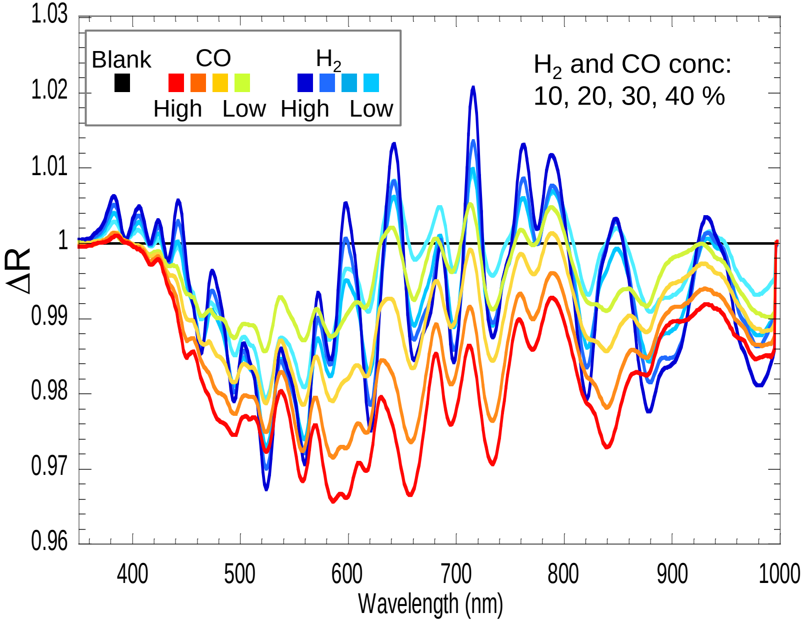
Our approach:
Multivariable photonic gas sensors

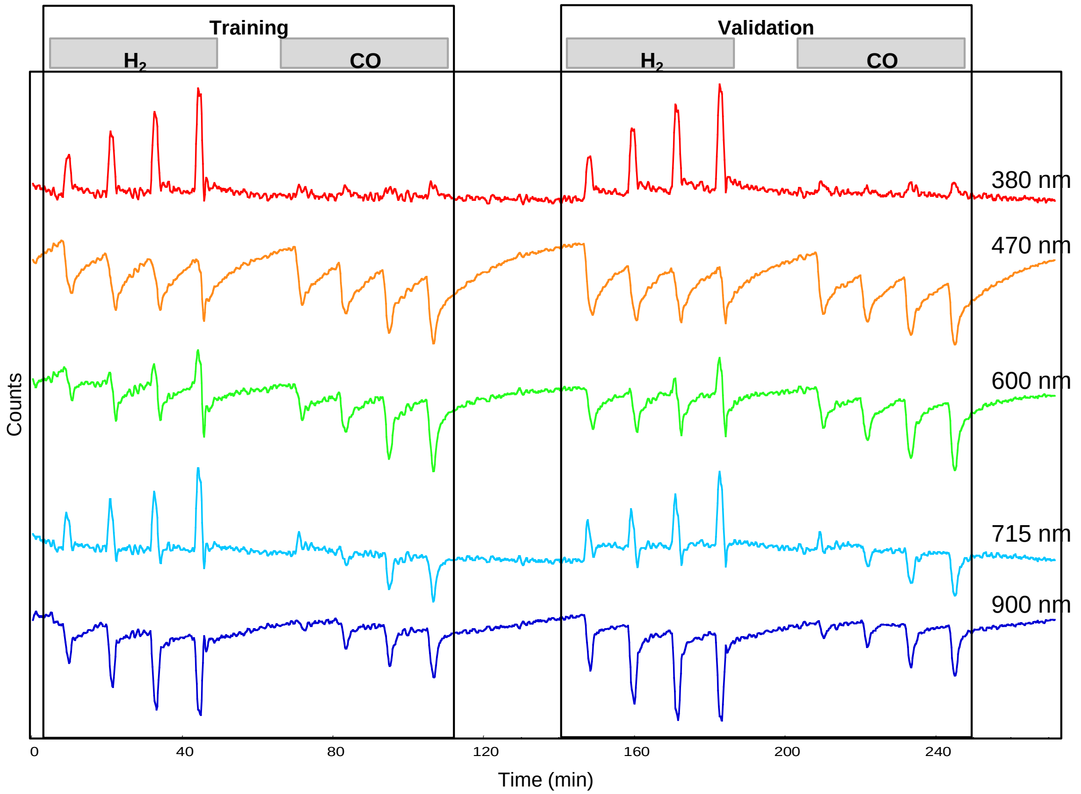


Real-time knowledge of H_2/CO ratio of anode tail gases:

- to allow control of efficiency of reforming process in the SOFC system
- to deliver a lower operating cost for SOFC customers

Response to H_2 and CO

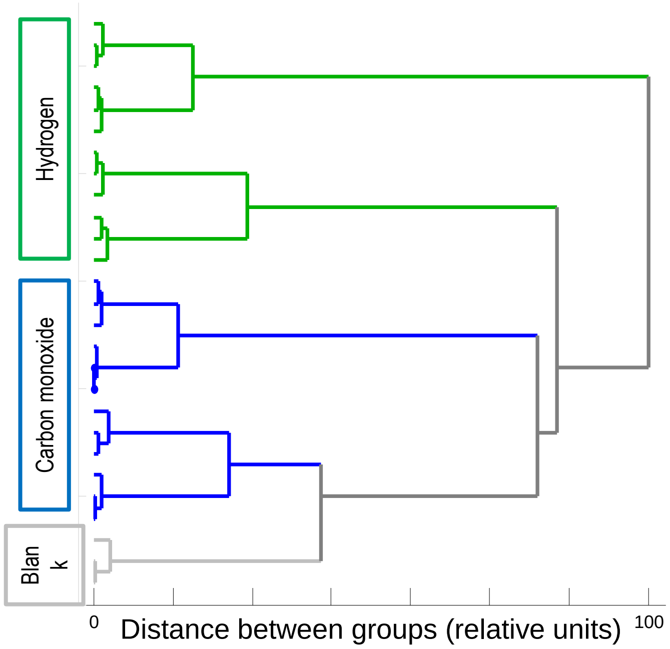




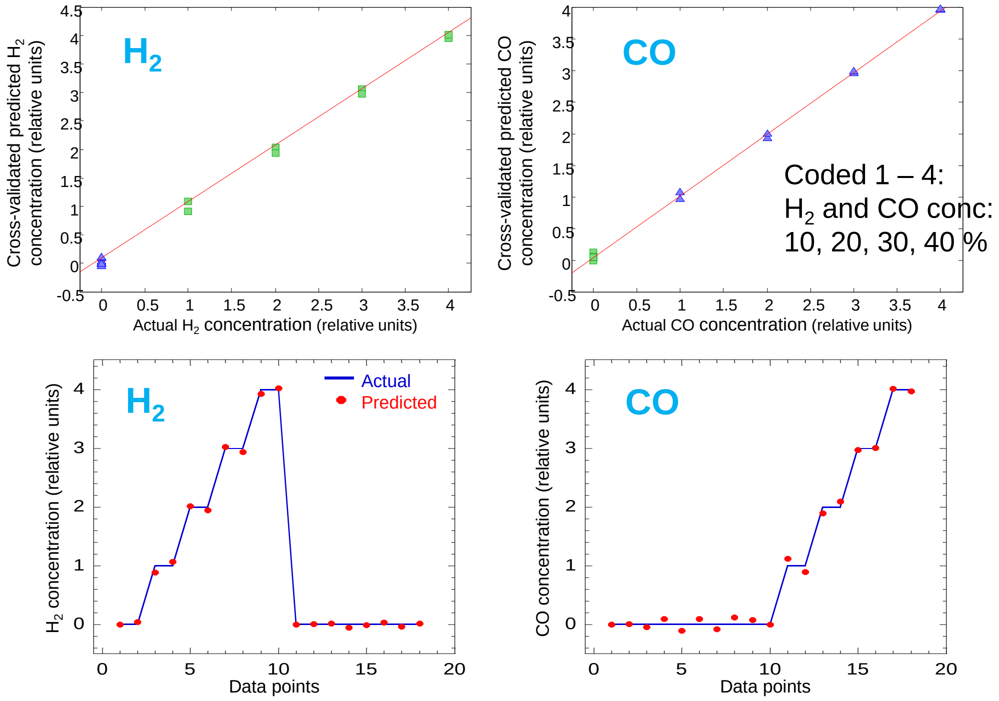
Spectral diversity of responses at different wavelengths allows discrimination of H_2 and CO gases

Differentiation between to H_2 and CO

Hierarchical cluster analysis



Cross validated prediction of H_2 and CO

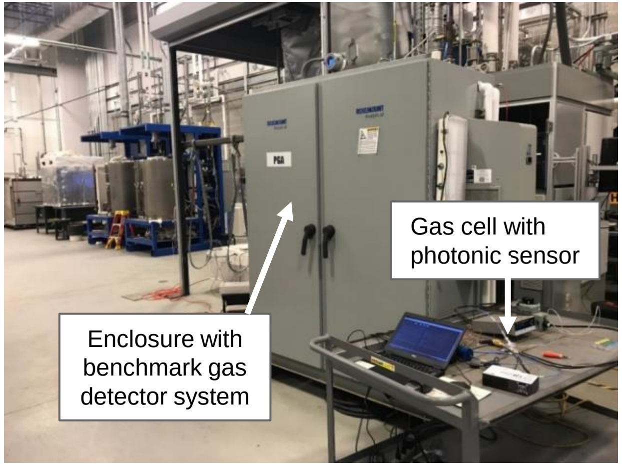


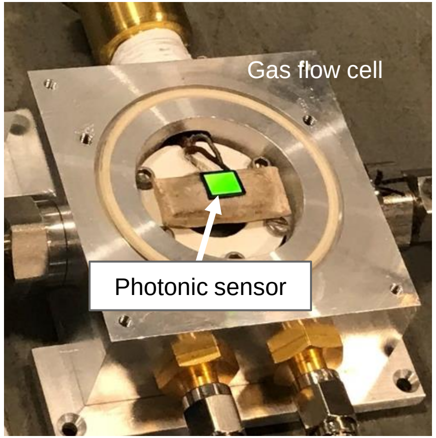
Resolution between individual concentrations of H_2 and CO

Field tests of nanostructured sensors at GE Fuel Cells

Example of two SOFCs

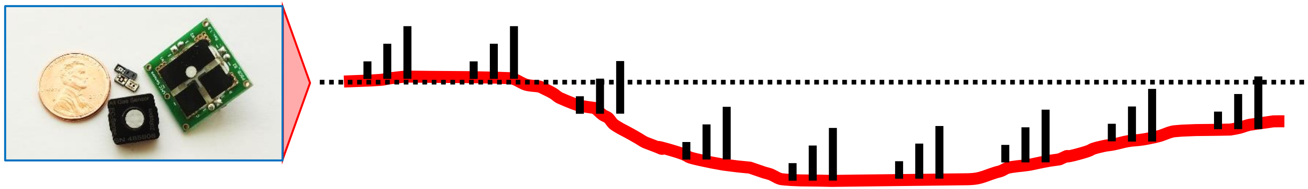
Benchmark and sensor systems



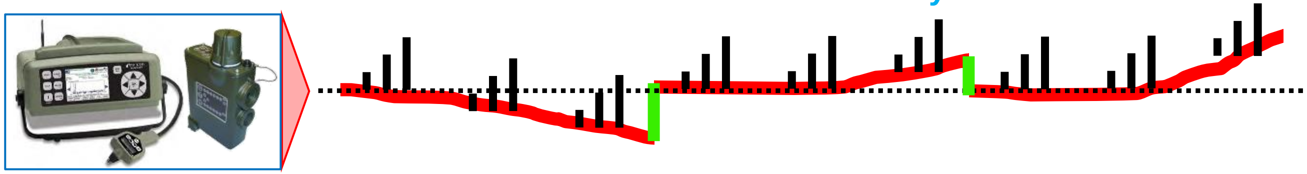


Effects of baseline drift in three categories of instruments

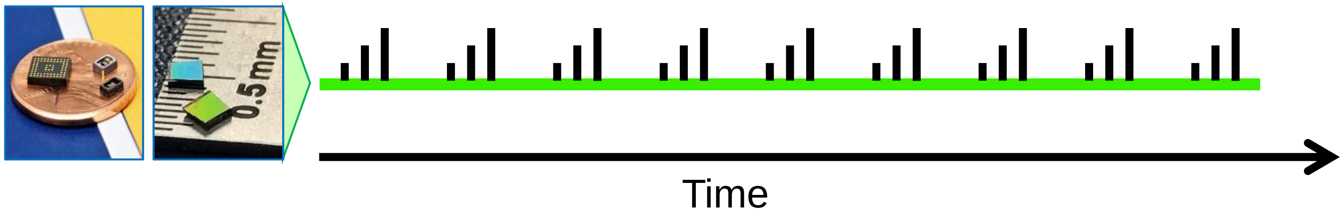
Undetected accuracy loss of single-output gas sensors



Periodic resets and/or re-calibrations of traditional analytical instruments



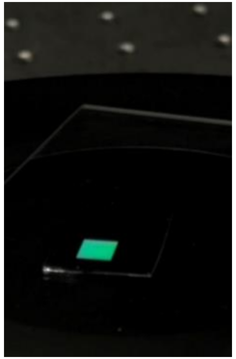
Concept of multivariable sensors with a self-correction for effects of baseline drift

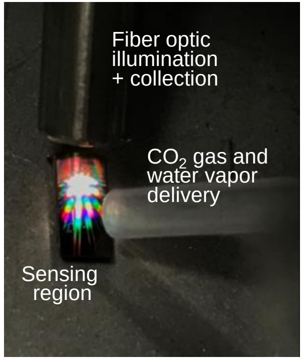


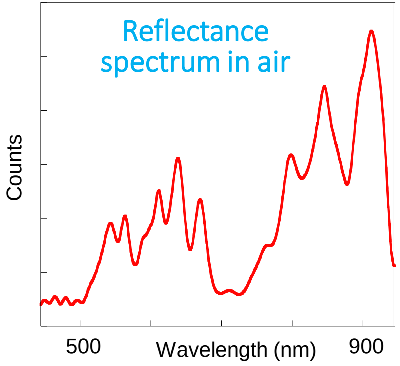
Potyrailo, R. A. *et al. Appl. Spectrosc.* **2023**

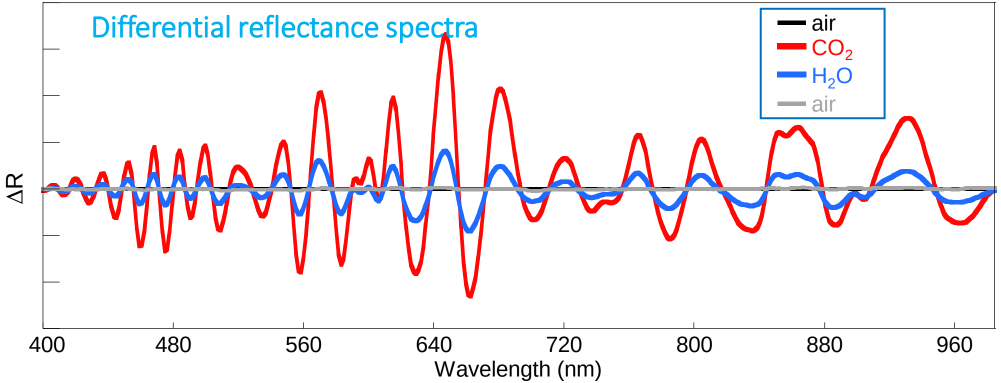
Resolution of mixtures of CO_2 with water vapor using multivariable gas sensor

White-light illumination of sensor





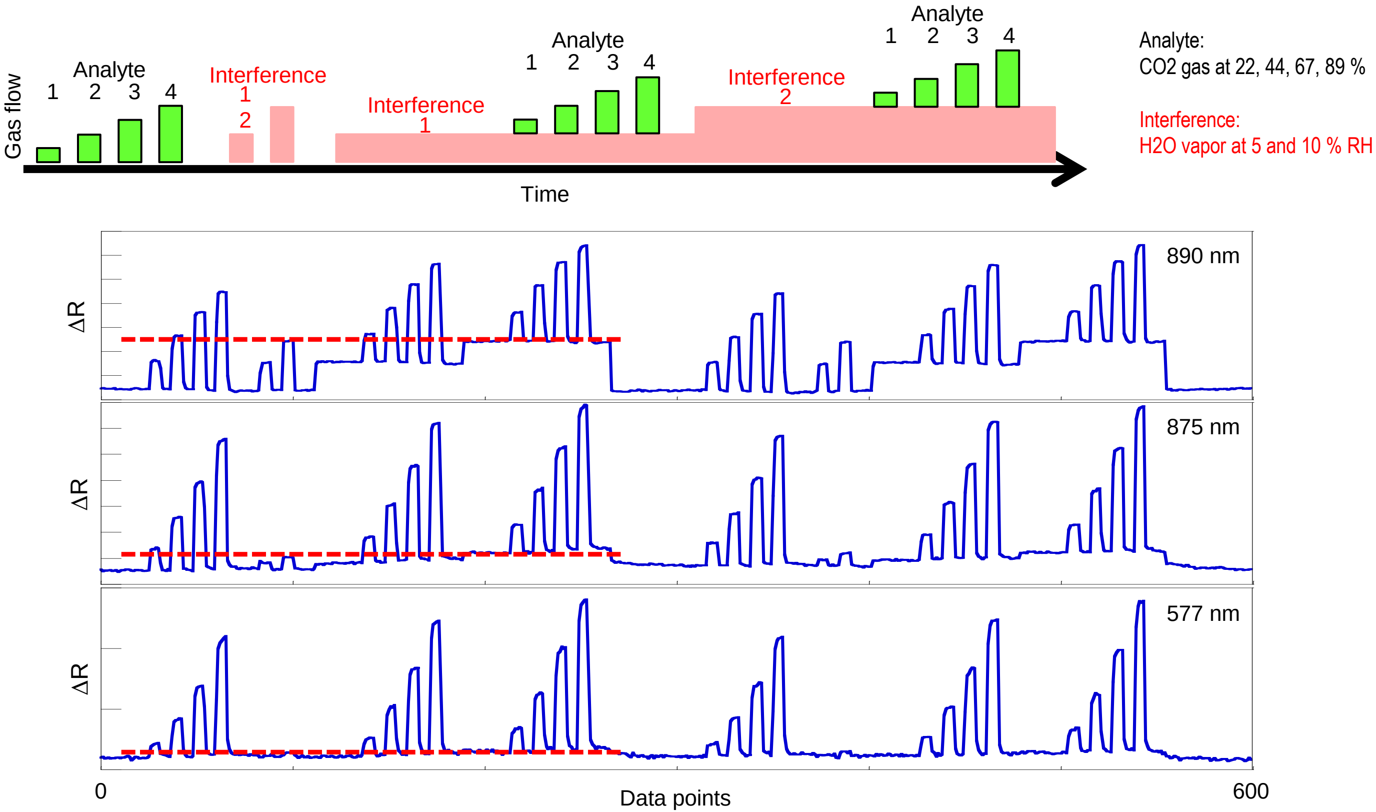




GE VERNOVA IEEE Sensors Council

Potyrailo, R. A. *et al. Appl. Spectrosc.* **2023**

Bioinspired photonic gas sensing: elimination of drift



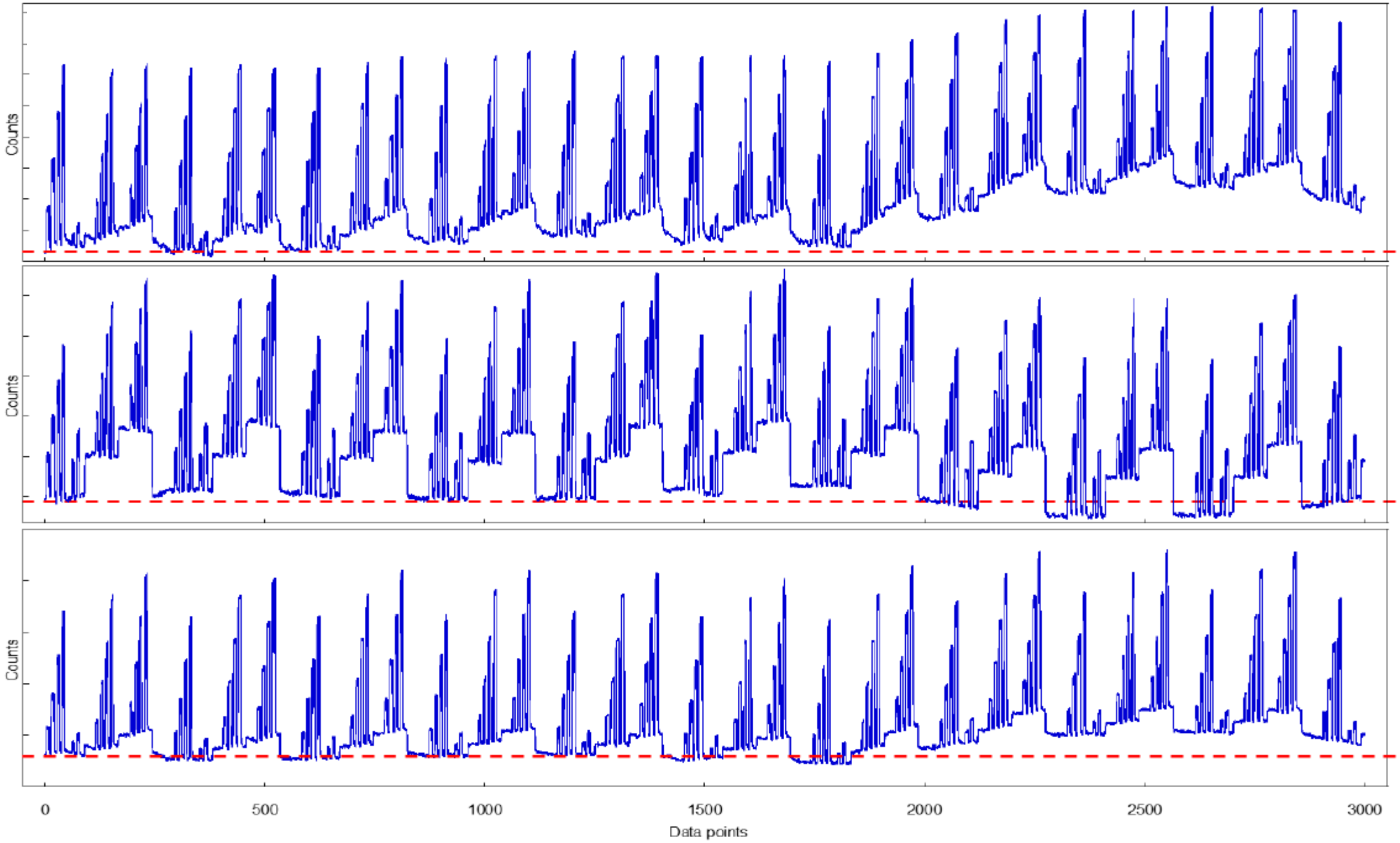
Analyte:
CO_2 gas at 22, 44, 67, 89 %

Interference:
H_2O vapor at 5 and 10 % RH

Excellent short term response for selective analyte quantitation

Potyrailo, R. A. *et al. Appl. Spectrosc.* **2023**

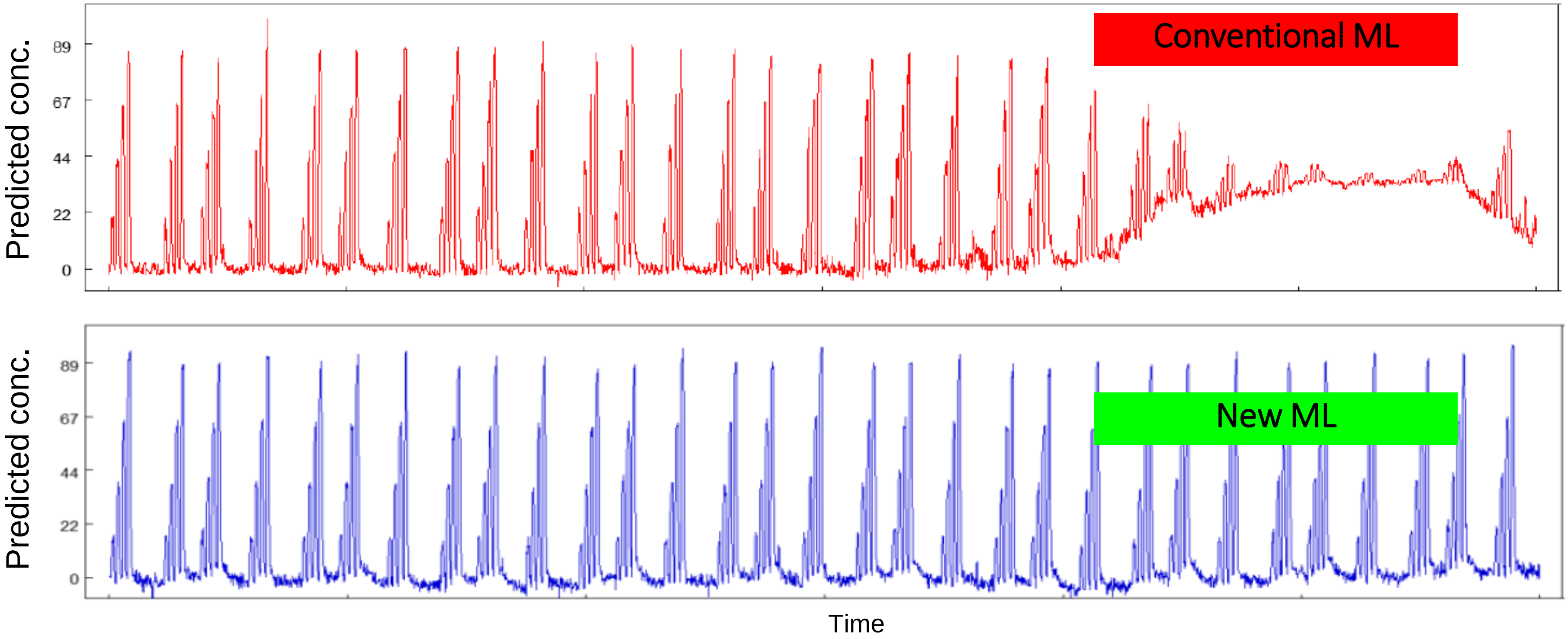
Long-term response: analyte, interference, their mixtures



Long term response exhibits strong baseline drift

Potyrailo, R. A. *et al. Appl. Spectrosc.* **2023**

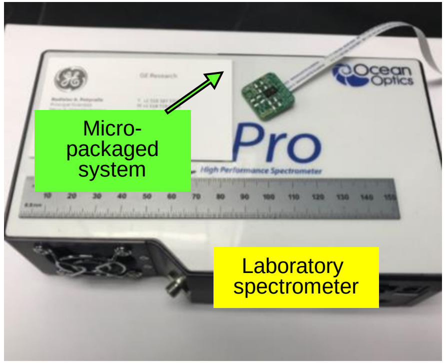
Sensor stability boost using advanced data analytics (a.k.a. machine learning, ML)



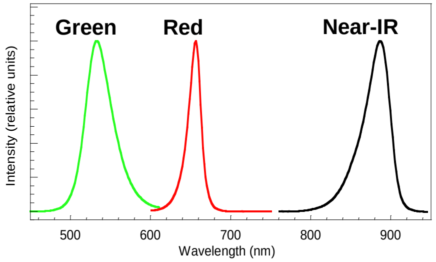
Sensor stability boost using machine learning based on transducer outputs

Potyrailo, R. A. *et al. Appl. Spectrosc.* **2023**

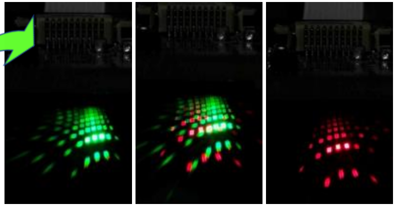
Toward design of nanostructured materials for operation with pulse oximeter LEDs

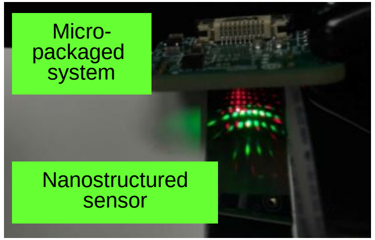


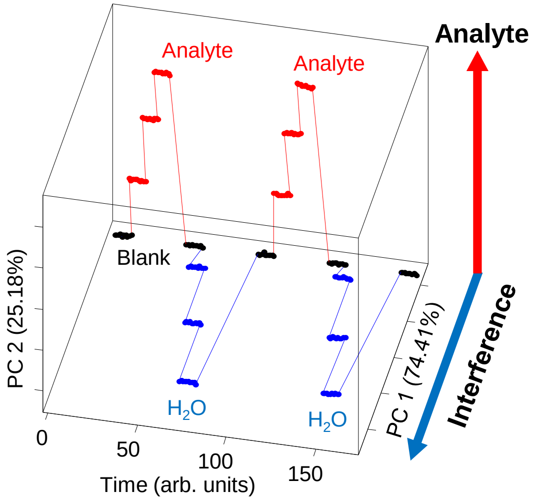
Spectra of LEDs



Pulsed operation of LEDs



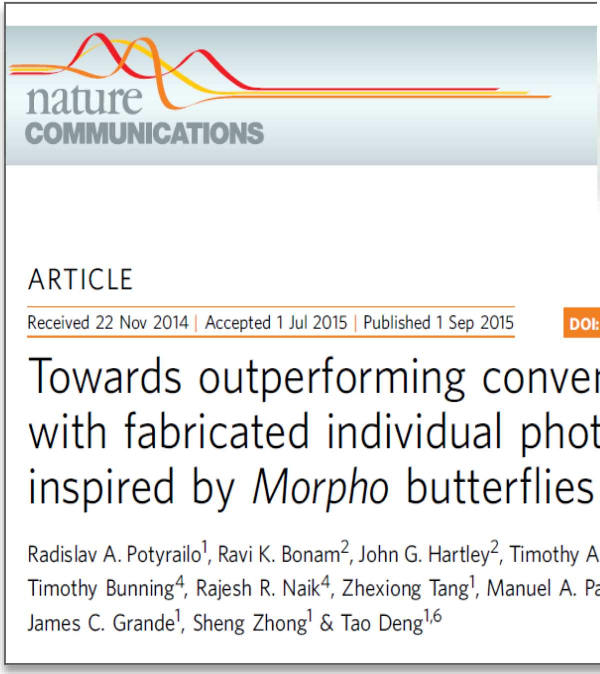




Potyrailo, et *al. From Natural to Fabricated Gas Sensing Photonic Nanostructures: Unexpected Discoveries and Societal Impact*. (AVS 69th International Symposium & Exhibition, Portland, OR, Nov 5 - 10, Paper 78421, **2023**)

Rejection of interference (humidity) on par with more bulky multivariable sensor systems

New spectrometer architectures



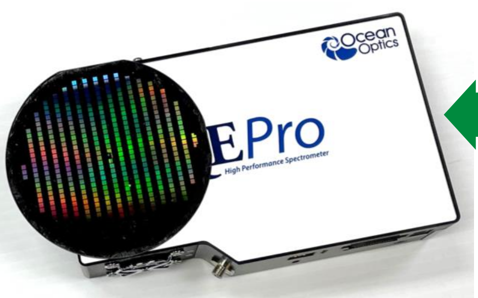
ARTICLE

Received 22 Nov 2014 | Accepted 1 Jul 2015 | Published 1 Sep 2015

DOI: 10.1038/ncomms8959 OPEN

Towards outperforming conventional sensor arrays with fabricated individual photonic vapour sensors inspired by *Morpho* butterflies

Radislav A. Potyrailo[1], Ravi K. Bonam[2], John G. Hartley[2], Timothy A. Starkey[3], Peter Vukusic[3], Milana Vasudev[4,5], Timothy Bunning[4], Rajesh R. Naik[4], Zhexiong Tang[1], Manuel A. Palacios[1], Michael Larsen[1], Laurie A. Le Tarte[1], James C. Grande[1], Sheng Zhong[1] & Tao Deng[1,6]



Potyrailo et. al., *Nature Communications* **2015**

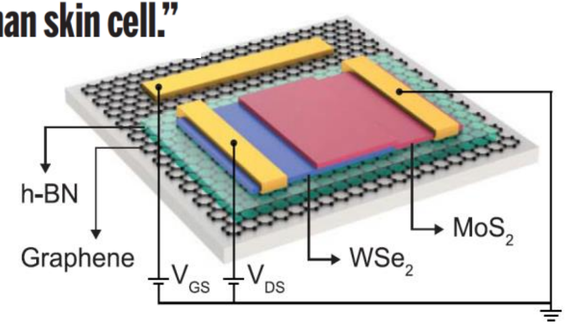
SPECTROSCOPY

An ultraminiaturized spectrometer

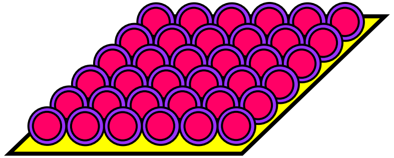
Scaling down spectrometers could allow their application in consumer devices

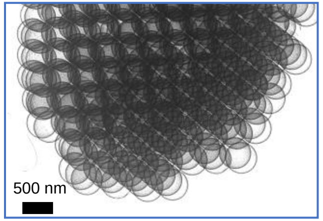
"The device has a footprint of 22 μm by 8 μm, which is smaller than the average human skin cell."

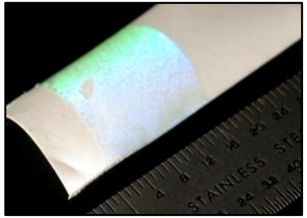
Yoon et al., *Science* 378, 296–299 (**2022**)

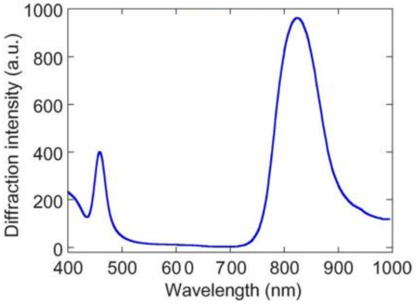


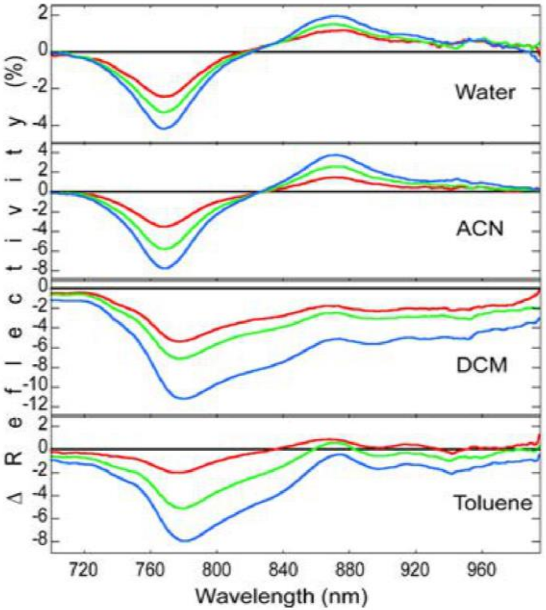
3-D dispersion
in bio-inspired core/shell photonic colloidal crystal sensors

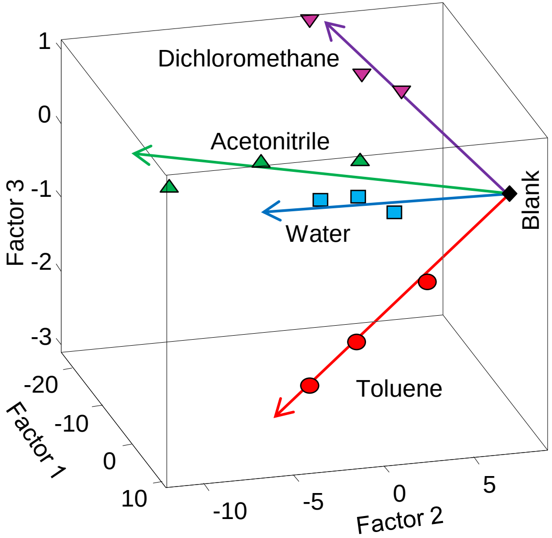












Sensor selectivity is based on optical lattice constant of colloidal crystal with cores and shells of nanospheres responding to diverse vapors

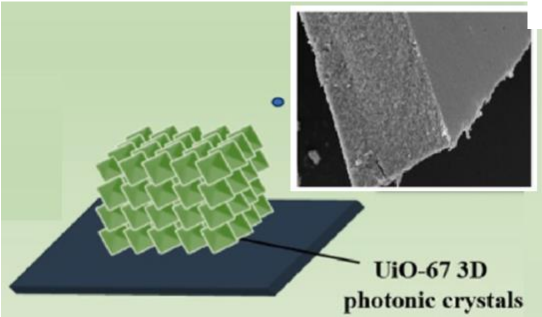
Potyrailo, et al., IEEE Sens. J., 2008, 8, 815–822

Part-per-billion gas detection with bio-inspired protonic crystals

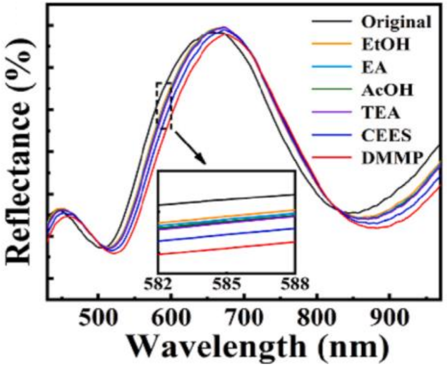
Metal organic framework

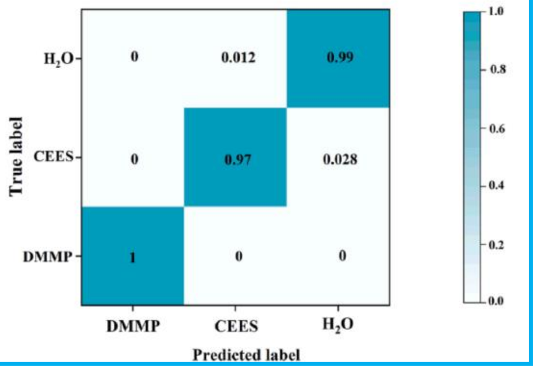
DMMP simulant

LOD
12- 43 ppb



Wang et al., *Talanta* **2024**, 126383

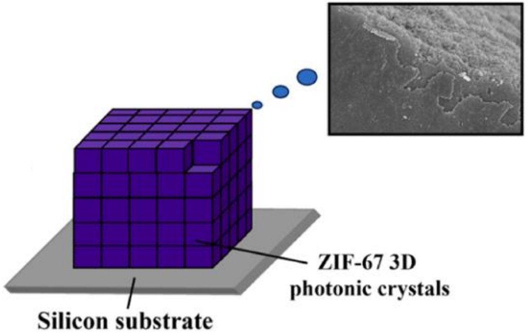




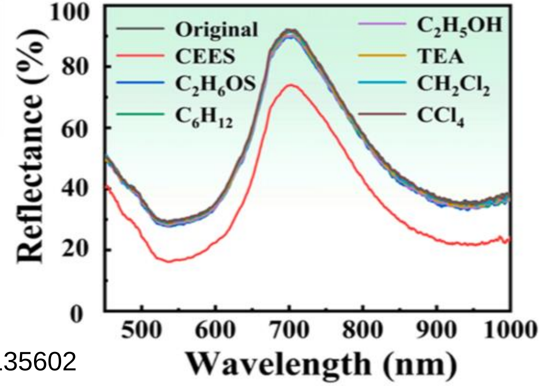
Zeolite

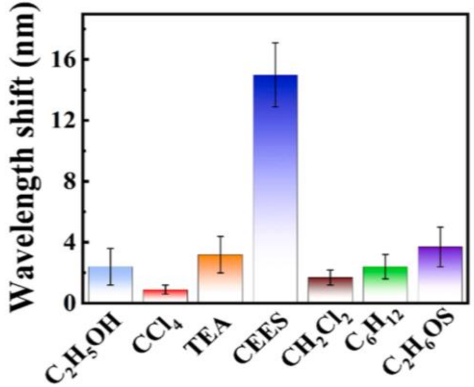
CEES simulant

LOD
19- 22 ppb



Wang et al., *Sens. Actuators B* **2024,** 409, 135602

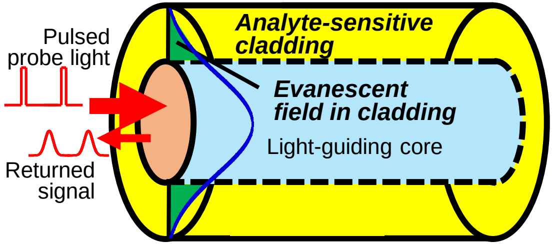




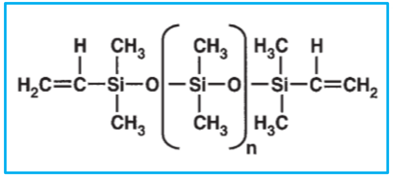
DMMP = dimethyl methylphosphonate
CEES = 2–chloroethyl ethyl sulfide

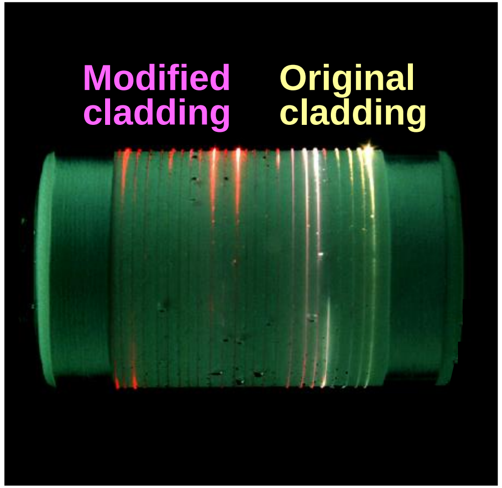
DMMP and CEES are chemical warfare agent (CWA) simulants

Multi-gas sensing with chemically modified fiber-optic cladding

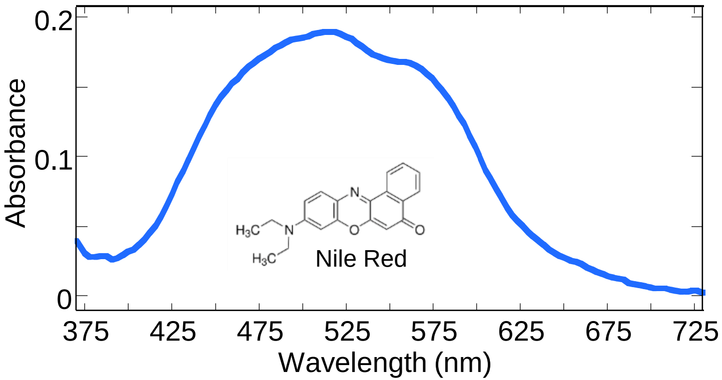


Silicone cladding of plastic-clad silica (PCS) fiber

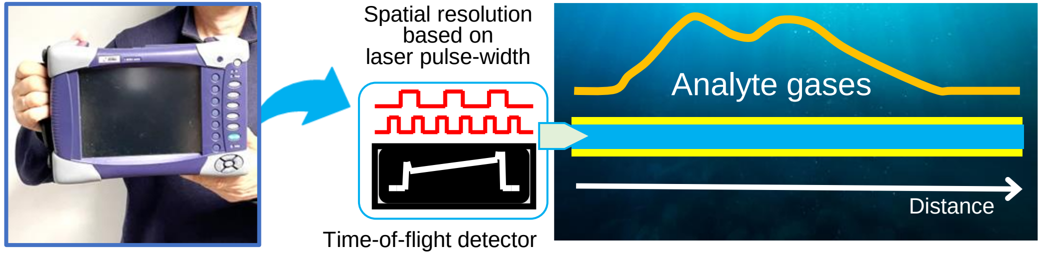




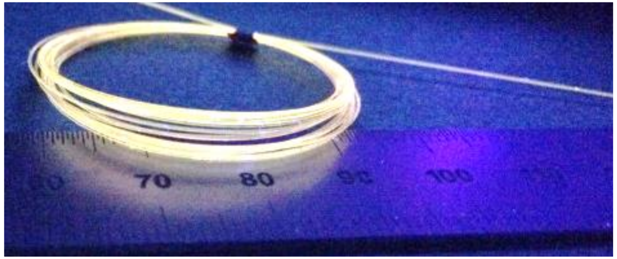
Evanescent-wave absorption spectrum of PCS optical fiber with chemically modified cladding



Optical readout for spatially resolved gas detection along the fiber



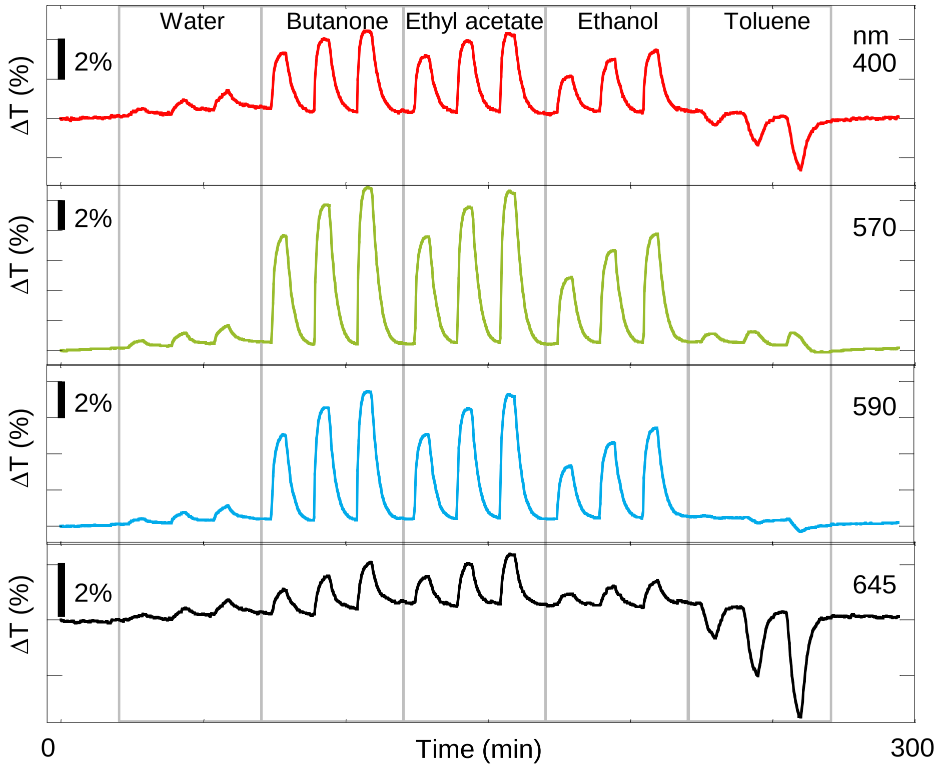
Coiled PCS optical fiber with chemically modified cladding

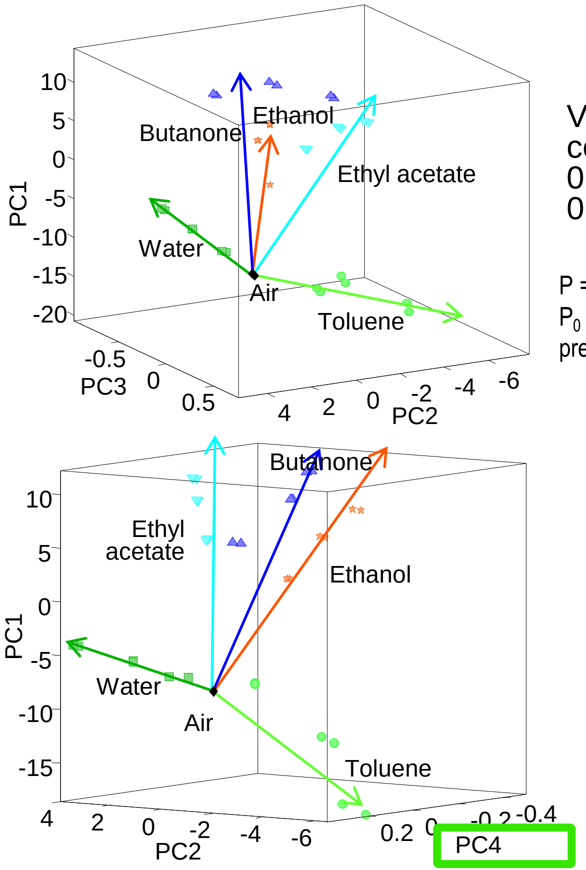


Sensing mechanism for multi-analyte detection: polymer interactions and reagent interactions with high-order modes

Potyrailo, *ISOEN* **2024**, 4092

4-D dispersion of response of fiber-optic sensor to five vapors





Vapor concentrations: 0.25, 0.50, 0.75 P/P_0

P = vapor partial pressure
P_0 = saturated vapor pressure

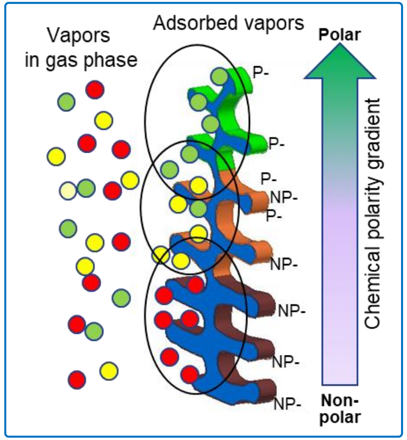
Wavelength-based diversity of responses to volatiles: different relative intensities and different directions

Potyrailo, *ISOEN* **2024**, 4092

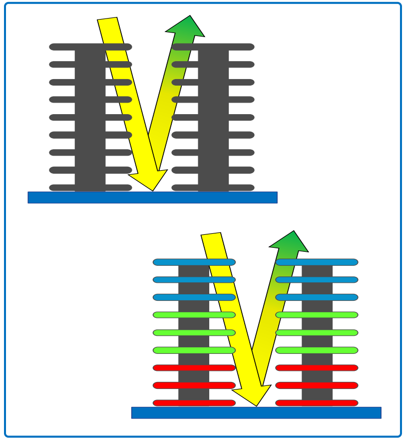
Summary: Photonic multivariable multi-gas sensors

- Developed theoretical understanding of exquisite multi-vapor differentiation by natural *Morpho* nanostructures
- Developed design rules of nano-structured sensors for multi-gas detection at room and high (300C) temperatures
- Implemented diverse nanofabrication techniques to build photonic nanostructures with spatial materials control

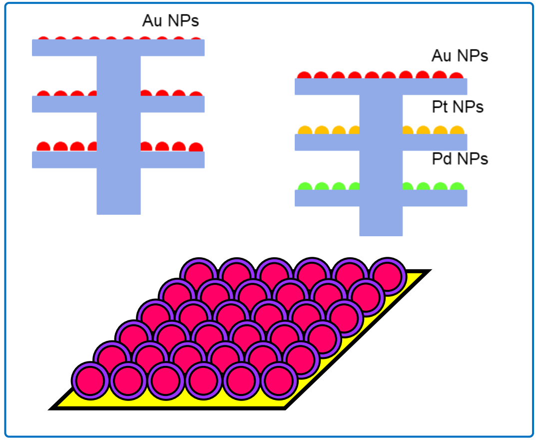
Theoretical understanding



Design rules of nano-structured sensors



Spatial materials control



Summary: Photonic multivariable multi-gas sensors

Performance capabilities

Selectivity:
highest response dispersion among multivariable sensors

Selectivity:
outperformed gas sensor arrays in side-by-side tests

Sensitivity:
part-per-million,
part-per-billion

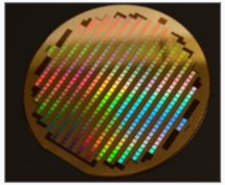
Multiple gases:
quantitation with a single sensor

Cost-effective fabrication

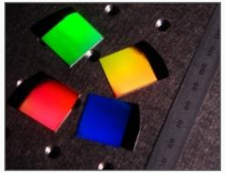
Photonic Integrated Circuits
- Emerging methodology
- Estimated cost per 100 mm^2 chip
  1 M chips/year = $500
  10 B chips/year = $0.2

Wafer-level system fabrication:
- Integrated tunable light source
- Gas sensing nanostructure
- Dispersive grating element
- Array detector
- Conditioning electronics

Wafer-level fab



Wafer-level fab

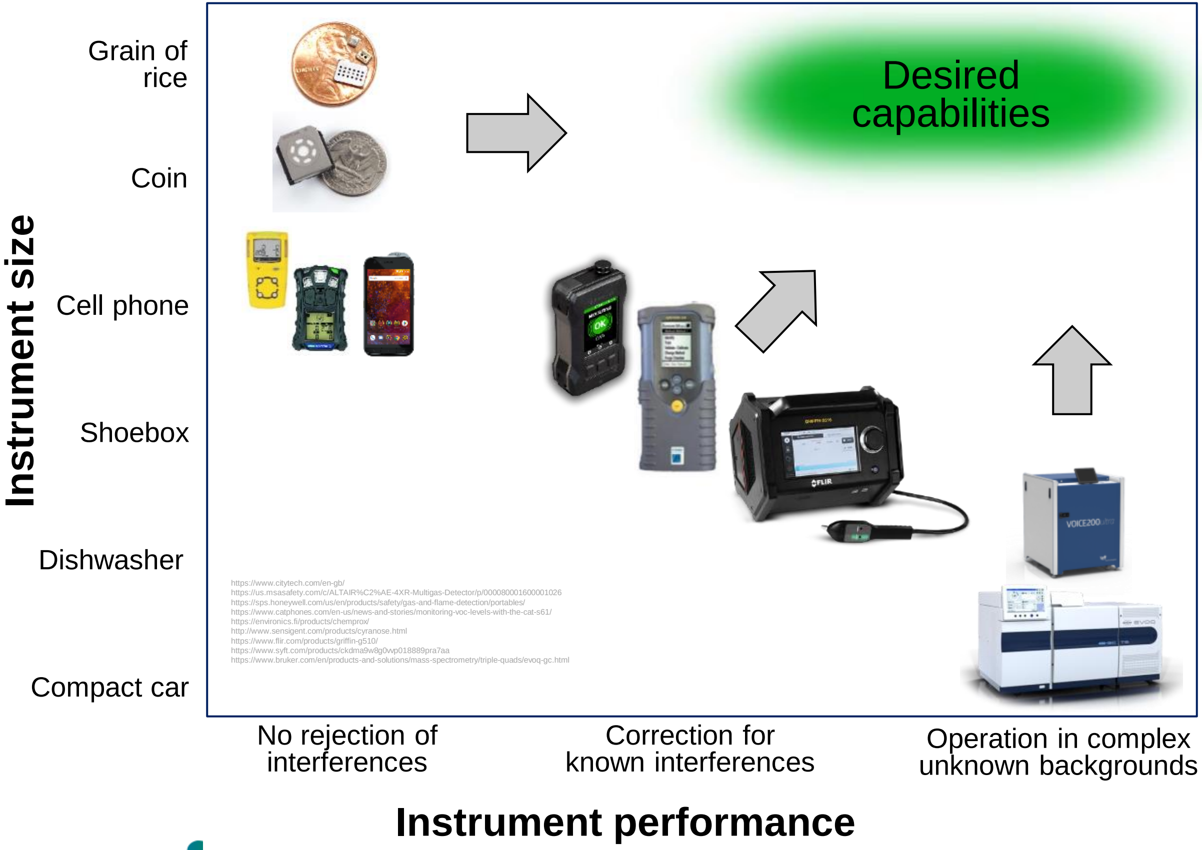


Examples of potential applications
for industrial, consumer, healthcare, environmental fields:

- Emissions monitoring at power plants
- Food and beverage safety monitoring
- Water purification testing
- Breath analysis for disease detection
- Wound healing assessment

Our vision toward ideal desired gas sensor capabilities:

(1) Develop new sensing principles to reach performance of traditional analytical instruments



US EPA Climate Adaptation Plans
https://www.epa.gov/climate-adaptation/climate-adaptation-plans

NASA Mitigation and Adaptation | Solutions – Climate Change
https://climate.nasa.gov/solutions/adaptation-mitigation/

FEMA NPB Climate Change Response and Recovery Planning Guidance
https://www.fema.gov/sites/default/files/documents/fema_response-recovery_climate-change-planning-guidance_20230630.pdf

US DoD Tackling the Climate Crisis
https://www.defense.gov/spotlights/tackling-the-climate-crisis/

DoD MEETING THE CLIMATE CHALLENGE
https://comptroller.defense.gov/Portals/45/Documents/defbudget/FY2023/FY2023_Meeting_the_Climate_Challenge_J-book.pdf

USDA Climate Change Adaptation
https://www.usda.gov/oce/energy-and-environment/climate/adaptation#:~:text=The%20Action%20Plan%20for%20Climate,and%20operational%20and%20financial%20climate

ARPA-E Accelerating U.S. Energy Innovation
https://arpa-e.energy.gov/technologies/publications/arpa-e-accelerating-us-energy-innovation

Our vision toward ideal desired gas sensor capabilities:

(2) Less computing power by hardware design for edge-based data analytics

Sept 20, 2024

https://www.theguardian.com/environment/2024/sep/20/three-mile-island-nuclear-plant-reopen-microsoft


Three Mile Island nuclear reactor to restart to power Microsoft AI operations

Pennsylvania plant was site of most serious nuclear meltdown and radiation leak in US history in 1979

The Three Mile Island in 2011. Its owner, Constellation Energy, will restart Unit 1, the reactor it closed in 2019. Photograph: Bradley C Bower/AP

Cross-pollination of electronics **+** mathematics **=**
Toward performance boost in ***multivariable*** gas sensors

Thank you !

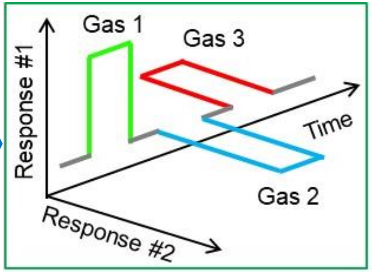
Acknowledgements

Radislav Potyrailo potyrailo@ge.com

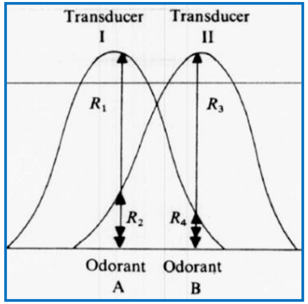
R. A. Potyrailo 2023 69

Original concept of sensor arrays: E-Nose

Air sample → **Sensing material** •Organic •Inorganic •Biological •Composite → **Transducer** •Electrical energy •Mechanical energy •Thermal energy •Radiant energy → **Data analytics** •Unsupervised •Supervised •Qualitative •Quantitaive →

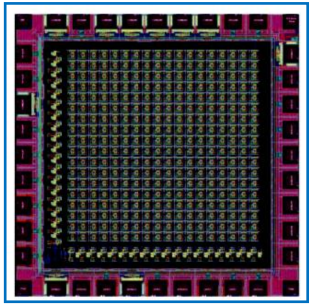


Three-sensor array



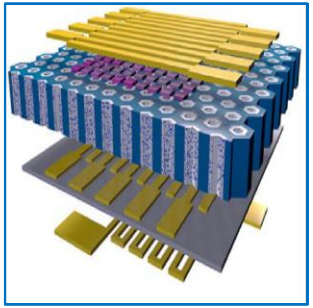
Persaud, Dodd, *Nature* **1982**

324



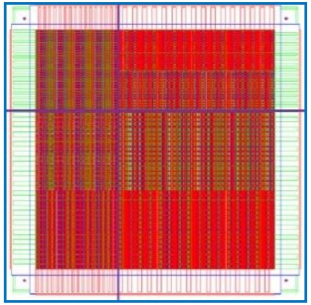
Dickson et al., *IEEE Symp. Circ. Syst.* **2000**

100 x 100 = 10,000



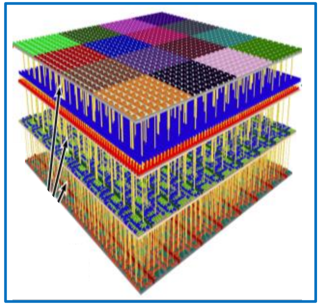
Wang et al., *Nature Electronics* **2024**

2^16 = 65,536



Beccherelli et al., *Sens. Actuat. B* **2010**

2^20 = 1,000,000+



Shulaker, *et al.*, *Nature* **2017**

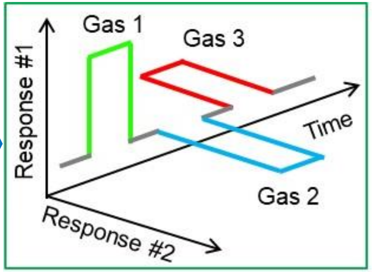
Concept of sensor arrays: E-Nose 2.0

Air sample

Sensing material
- Organic
- Inorganic
- Biological
- Composite

Transducer
- Electrical energy
- Mechanical energy
- Thermal energy
- Radiant energy

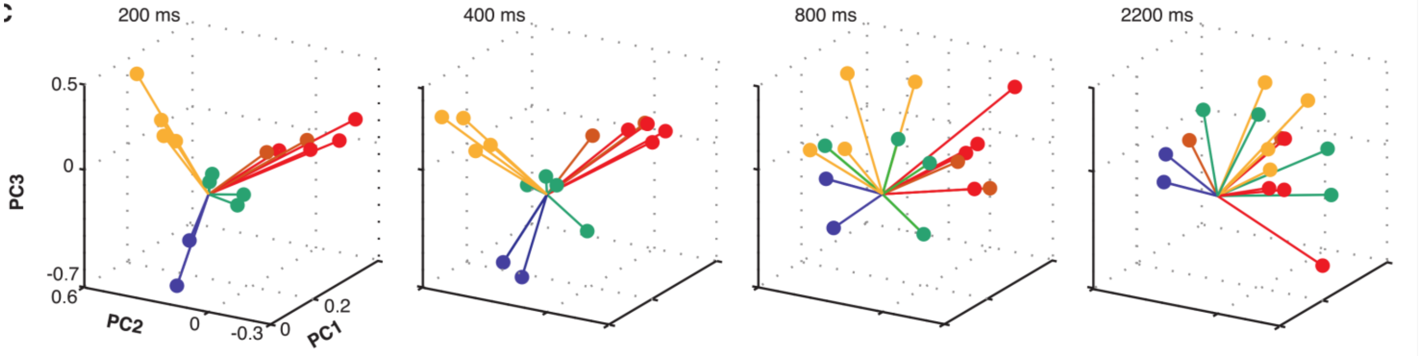
Data analytics
- Unsupervised
- Supervised
- Qualitative
- Quantitaive



Dynamic / modulated sample introduction and differentiation

Mitral cells in the olfactory bulb in zebrafish:

Temporal separation of odors starting from families (200 ms) to individual odors(2200 ms)



Friedrich, R. W.; Laurent, G. Dynamic optimization of odor representations by slow temporal patterning of mitral cell activity, *Science* **2001**, 291, (5505), 889-894

Concept of sensor arrays: E-Nose 2.0

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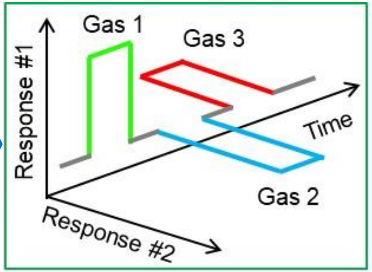
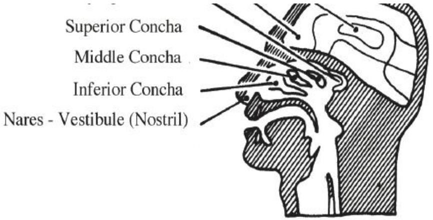


Regeneration of sensing material (receptors)

"…olfactory receptors renew themselves every thirty days"



Science of Smell Part 1: Perception and Physiological Responses to Odors

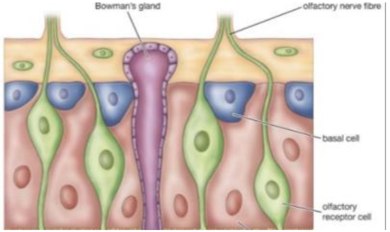
https://porkgateway.org/resource/science-of-smell-part-1-perception-and-physiological-responses-to-odors/

"Scent cells are renewed every 30 to 60 days"

10 Incredible Facts About Your Sense of Smell, 2014

https://www.everydayhealth.com/news/incredible-facts-about-your-sense-smell/

"In humans the receptor cells are replaced about every 60 days"



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https://www.britannica.com/science/chemoreception/Smell

Concept of sensor arrays: E-Nose 2.0

Air sample

Sensing material
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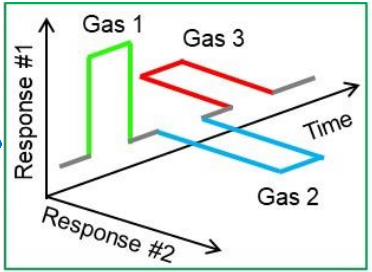
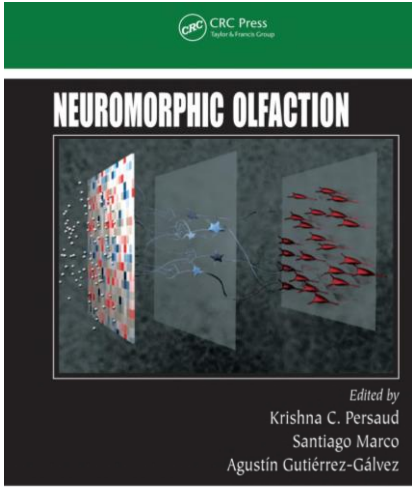
Data analytics
•Unsupervised
•Supervised
•Qualitative
•Quantitaive



Neuromorphic olfaction



Neuromorphic Olfaction
Edited By
Krishna C. Persaud,
Santiago Marco,
Agustin Gutierrez-Galvez,
CRC Press, **2013**