

# C-PASS

Conference on Photonics  
for Advanced Spectroscopy and Sensing



## CONFERENCE ON PHOTONICS FOR ADVANCED SPECTROSCOPY AND SENSING

ENVIRONMENTAL AND BIO-MEDICAL APPLICATIONS SENSING,  
INDUSTRIAL PROCESS MONITORING AND AGRI-FOOD ANALYSIS

14 - 19 SEPTEMBER 2025

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**C-PASS 2025** is the second edition of the international conference series on **Photonics for Advanced Spectroscopy and Sensing**, held on **14-19 September 2025** in **Calaserena Resort, nearby Cagliari, Italy**. It aims to bring together researchers from both industrial and academic research laboratories to stimulate new research initiatives in the fields of **integrated photonics, lasers, optical spectroscopy and sensing in the near- and mid-infrared spectral regions**.

## Topics

- Gas and liquid sensing and spectroscopy
- Photoacoustic and photothermal gas sensing
- Integrated photonics for sensing and spectroscopy
- Sensor phenomenology, modeling and evaluation
- Emerging sensor technologies and applications
- Novel mid and near-IR sources for gas and liquid sensing
- Optical sensor systems: signals, processing and interfaces
- Optical sensors for agrifood analysis and industrial applications
- Environmental and bio-medical sensors, new instrumentation and methodology
- VOCs and particulate detection

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Sunday Sept. 14 <sup>th</sup>		Monday Sept. 15 <sup>th</sup>		Tuesday Sept. 16th		Wednesday Sept. 17th		Thursday Sept. 18th		Friday Sept. 19th	
		Metamaterials and Metasurfaces for Spectroscopy		Advanced Spectroscopic Techniques		Bio-medical Applications - Sponsored by Project Brief		Integrated Silicon Photonics		Sensing for Security and Food Applications - Sponsored by project EVOQUE	
09:00 - 09:15		Opening: V. Spagnolo, W. Whelan Curtin, L. Dong, S. Cristescu		09:00 - 09:30		09:00 - 09:20		09:00 - 09:30		09:00 - 09:20	
09:15 - 09:45		C. Sirtori- Metamaterial Enhanced Unipolar Quantum Optoelectronics		09:30 - 09:50		09:20 - 09:40		09:30 - 09:50		09:20 - 09:35	
09:45 - 10:05		M. Belkin - Tunable continuous-wave 1-11 THz light sources based on difference-frequency mixing in intersubband polaritonic metasurfaces		09:50 - 10:10		09:40 - 10:00		09:50 - 10:10		09:35 - 9:50	
10:05 - 10:20		A. Vorobev - Metasurfaces for the Mid-Infrared Spectroscopy Application		10:10 - 10:25		10:00 - 10:15		10:10 - 10:25		9:50 - 10:05	
10:20 - 10:35		G. Piscopo- Mid-IR Spatial Light Modulation Using Germanium Metamaterials		10:205 - 10:40		10:15 - 10:30		10:25 - 10:40		10:05 - 10:20	
10:40 - 11:00		Coffee Break		10:40 - 11:00		10:40 - 11:00		10:40 - 11:00		10:40 - 11:00	
		Novel Infrared Sources and Detectors		Photothermal and Photoacoustic Spectroscopy		Breath Analysis - Sponsored by Project D3-4Health		Industrial Applications		Spectroscopy for air pollutants detection - Sponsored by MAECI	
11:00 - 11:20		P. De Natale- Shaping Photon Statistics in Mid-Infrared Cascade Lasers		11:00 - 11:20		11:00 - 11:20		11:00 - 11:15		11:00 - 11:20	
11:20 - 11:35		R. De Palo - Laser-textured Quartz-Tuning-Forks as infrared photodetector		11:20 - 11:40		11:20 - 11:40		11:15 - 11:30		11:20 - 11:40	
11:35 - 11:50		A.P. Cantatore- Lithium Niobate Tuning Forks as piezoelectric transducers in Infrared Spectroscopy for gas sensing		11:40 - 12:00		11:40 - 12:00		11:30 - 11:45		11:40 - 11:55	
11:50 - 12:05		A. de Cedeira Oliveira - Ge-on-Si bias-tunable dual-band photodetector for solvent recognition		12:00 - 12:20		12:00 - 12:15		11:45 - 12:00		11:55 - 12:10	
12:05 - 12:20		F. Pages- New capacitive MEMS design for photoacoustic gas sensing		12:20 - 12:35		12:15 - 12:30		12:00 - 12:15		12:10 - 12:25	
12:20 - 12:35		J. Pelini- Exploiting unconventional silicon-based Micro-Electro-Mechanical systems for high-sensitivity cantilever-enhanced photoacoustic spectroscopy		12:35 - 12:50		12:30 - 12:45		12:15 - 12:30		12:25-12:40	
12:50 - 14:00		Lunch		12:50 - 14:00		12:50 - 14:00		12:50 - 14:00		12:50 - 14:00	
		Optical Sensing and Spectroscopy				Quartz and Cantilever-Enhanced Photoacoustic Spectroscopy					
14:30 - 14:50		R. Krebbers - Spectroscopic applications of novel ultra-broadband, mid-infrared IDFG-based sources		14:30 - 14:50		14:30 - 14:50		14:30 - 14:50		14:30 - 14:50	
14:50 - 15:10		F. Wang- Multidimensional optical information detection		14:50 - 15:10		14:50 - 15:10		14:50 - 15:10		14:50 - 15:10	
15:10 - 15:25		D. Barberio- Raman spectroscopy for Clostridia produced hydrogen detection in milk		15:10 - 15:25		15:10 - 15:25		15:10 - 15:25		15:10 - 15:25	
15:25 - 15:40		H. Fei - Topological ring resonator for refractive index sensing at telecommunication wavelength		15:25 - 15:40		15:25 - 15:40		15:25 - 15:40		15:25 - 15:40	
15:40 - 15:55		E. Petronijevic - Photo-acoustics meets nanoplasmonics: widely tunable photo-acoustic spectroscopy on commercial nanostructured samples		15:40 - 15:55		15:40 - 15:55		15:40 - 15:55		15:40 - 15:55	
15:55 - 16:10		C. Birot - Wavelength Modulation Spectroscopy for the study of nitrogen oxide concentration after electric discharges simulating lightning		15:55 - 16:10		15:55 - 16:10		15:55 - 16:10		15:55 - 16:10	
18.00-19.30		WELCOME PARTY		19.30-21.00		19.30-21.00		19.30-21.00		19.30-21.00	
19.30-21.00		DINNER		DINNER		DINNER		SOCIAL DINNER			

# Metamaterials and Metasurfaces for Spectroscopy



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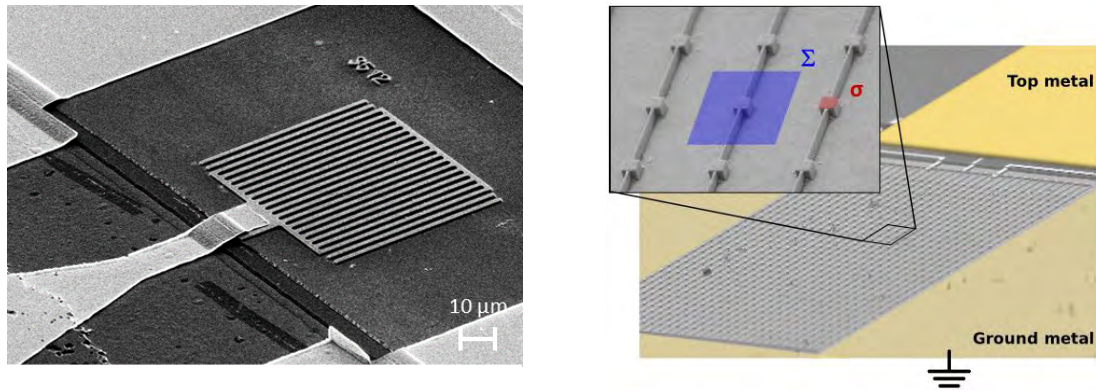
# Metamaterial Enhanced Unipolar Quantum Optoelectronics

Carlo Sirtori<sup>1</sup>, Marta Mastrangelo<sup>1</sup>, Jihye Baik<sup>1</sup>, Baptiste Chomet<sup>1</sup>, Angela Vasanelli<sup>1</sup>

*1. Laboratoire de Physique de l'ENS, École Normale Supérieure, Université PSL, CNRS, 75005 Paris, France*

**Short abstract:** Metamaterials play a major role in optoelectronic and photonic devices due to their ability to enhance light-matter interaction. I will show how metallic structures made of patch antennae found the bases for metamaterials that greatly improve the performances of detectors, modulators and lasers.

Unipolar quantum devices rely on optical transitions between electronic states confined in the conduction band of semiconductor quantum wells. They operate in the midinfrared wavelength range ( $3\ \mu\text{m} < \lambda < 15\ \mu\text{m}$ ) and are suited for several applications, namely, spectroscopy, light detection and ranging (Lidar), and free space communications. An important characteristic of unipolar devices is that they are intrinsically fast with bandwidth up to 100 GHz [1], due to the very short lifetime of the electrons in the excited state. Detectors [2], Stark modulators [2] and quantum cascade lasers form a versatile platform, called Unipolar Quantum Optoelectronics (UQO). In this presentation it will be explained how the performances of UQO devices can be greatly improved by inserting them into metamaterials [3,4]. It will be also discussed the principles of the microcavity arrays of patch antenna devices and the characterisation of the metamaterial devices.



**Fig. 1** Scanning Electron Microscope (SEM) image of the patch-antenna array metamaterials. Left panel: high frequency infrared modulators at  $9\ \mu\text{m}$  with a bandwidth of 20 GHz. Right panel: quantum cascade emitter. In this device the active region is embedded within double-metal cavities. Inset: a magnified view of the cavity array.

To illustrate the properties of these devices two exemplary devices will be described: Stark modulators and arrays of emitters. About modulators we will focus on their operation in the strong coupling regime and their dynamical properties which makes them ultrafast, with a theoretical bandwidth exceeding 150 GHz. Metamaterial emitters are a recent activity, in which we realise electroluminescent devices producing midinfrared light. These emitters produce a beam of highly collimated incoherent radiation with a relative broad spectrum. Moreover, their intensity has a strong enhancement given by the Purcell effect. Notably, all these peculiar physical properties descend directly from the microcavity arrays.

The use of metamaterials enables a significant enhancement of the functionality of unipolar devices. Owing to their efficient electromagnetic energy confinement, the antenna effect and the reduction of electrical area, they promote high-frequency photonic devices, with an enhanced radiative emission due to Purcell effect.

## References

- [1] P. Grant, R. Dudek, M. Buchanan, and H. Liu, *IEEE photonics technology letters* 18, 2218 (2006).
- [2] H. Dely, T. Bonazzi, O. Spitz, E. Rodriguez, D. Gacemi, Y. Todorov, K. Pantzas, G. Beaudoin, I. Sagnes, L. Li, A. G. Davies, E. H. Linfield, F. Grillot, A. Vasanelli, and C. Sirtori, *Laser & Photonics Reviews* 16, 2100414 (2022).
- [3] D. Palaferri, Y. Todorov, A. Bigioli, A. Mottaghizadeh, D. Gacemi, A. Calabrese, A. Vasanelli, L. Li, A. G. Davies, E. H. Linfield, F. Kapsalidis, M. Beck, J. Faist, and C. Sirtori, *Nature* 556, 85 (2018).
- [4] T. Bonazzi, H. Dely, P. Didier, D. Gacemi, B. Fix, M. Beck, J. Faist, A. Harouri, I. Sagnes, F. Grillot, A. Vasanelli, and C. Sirtori, *APL Photonics* 9, 110801 (2024)



# Tunable continuous-wave 1-11 THz light sources based on difference-frequency mixing in intersubband polaritonic metasurfaces

J. Krakofsky<sup>1</sup>, M.A. Rieder<sup>1</sup>, G. Boehm<sup>1</sup>, and M.A. Belkin<sup>1</sup>

*1. Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, Garching 85748, Germany*

**Short abstract:** We demonstrate intersubband nonlinear polaritonic metasurfaces designed to provide highly-efficient terahertz difference-frequency mixing in 1-11 THz spectral range. When pumped with two milliwatt-level continuous-wave mid-infrared lasers, the metasurfaces provide tunable radiation in the 1-10 THz spectral range with up to 20  $\mu$ W of continuous-wave power output in the 6-11 THz spectral range, outperforming by a large margin any other broadly-tunable terahertz sources at frequencies above 5 THz.

Tunable continuous-wave sources of coherent terahertz radiation are highly desired for a wide range of applications, including spectroscopy, microscopy, metrology, and radio-astronomy. While several suitable technologies exist in the 1-5 THz spectral range, the spectral range 5-11 THz is currently completely devoid of such sources with reasonable (at least  $\sim 1$   $\mu$ W) output powers. Here we demonstrate that intersubband nonlinear polaritonic metasurfaces [1,2] can be designed to provide highly-efficient terahertz difference-frequency generation (DFG) in 1-10 THz spectral range. When pumped with two milliwatt-level continuous-wave mid-infrared lasers, the metasurfaces provide tunable radiation in the 1-10 THz spectral range with up to 20  $\mu$ W of continuous-wave power output, outperforming by a large margin any other broadly-tunable terahertz sources at frequencies higher than 5 THz.

Figure 1(a) shows the experimental setup: two CW mid-infrared lasers operating in the 8-11  $\mu$ m wavelength range are focused onto the metasurface through a hole in a parabolic mirror. THz difference-frequency radiation is outcoupled from the metasurface in reflection and is collected by the parabolic mirror. Figure 1(b) shows the spectra of THz DFG for different mid-infrared laser pump wavelengths. Figure 1(c) shows the tuning performance of two metasurfaces – one optimized for terahertz generation in the range 4-6 THz and the other one optimized for terahertz generation in the range 8-11 THz. The data is given as the ratio of the THz output power to the product of mid-infrared pump powers. Laser pumping powers in the range 100-200 mW were used for the THz generation, no power saturation is observed for pumping powers up to 200 mW.

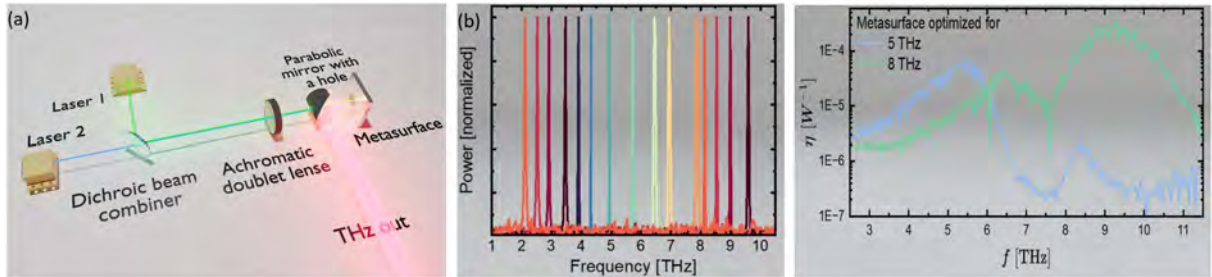


Fig. 1. (a) Schematic of the CW THz source based on intersubband polaritonic metasurfaces. Two CW mid-infrared lasers are focused onto the metasurface to generate THz output via difference-frequency generation. (b) The range of output frequencies of the THz source. (c) Mid-infrared-to-THz nonlinear conversion efficiency  $\eta$  as a function of THz output frequency for the two metasurfaces optimized for the best performance at 3-6 THz (blue line) and 6-11 THz (green line). The value of  $\eta$  is computed as the ratio of the THz output power to the product of mid-infrared pump powers.

This work was supported by the German Research Foundation (DFG) grant number 506515587.

## References

- [1] J.H. Krakofsky, R. Sarma, I. Brener, A. Alù, J. Lee, and M.A. Belkin, “Flat nonlinear optics with intersubband polaritonic metasurfaces,” *Nanophoton.*, advanced online publication (2025). <https://doi.org/10.1515/nanoph-2024-0742>
- [2] J. Lee, M. Tymchenko, C. Argyropoulos, P.-Y. Chen, F. Lu, F. Demmerle, G. Boehm, M.-C. Amann, A. Alu, and M.A. Belkin, “Giant nonlinear response from plasmonic metasurfaces coupled to intersubband transitions,” *Nature* **511**, 65–69 (2014). <https://doi.org/10.1038/nature13455>

# Metasurfaces for the Mid-Infrared Spectroscopy Application

A.S. Vorobev<sup>1,2</sup>, J.H. Mendoza-Castro<sup>3,4</sup>, G. Piscopo<sup>1,4</sup>, T. Piwonski<sup>2</sup>, G. Malvicini<sup>1,3</sup>, A. D'Orazio<sup>4</sup>,  
G. Magno<sup>2</sup>, B. Lendl<sup>1</sup> and L. O'Faolain<sup>3,4</sup>

1. Centre for Advanced Photonics and Process Analysis, Munster Technological University, T12 T66T, Cork, Ireland

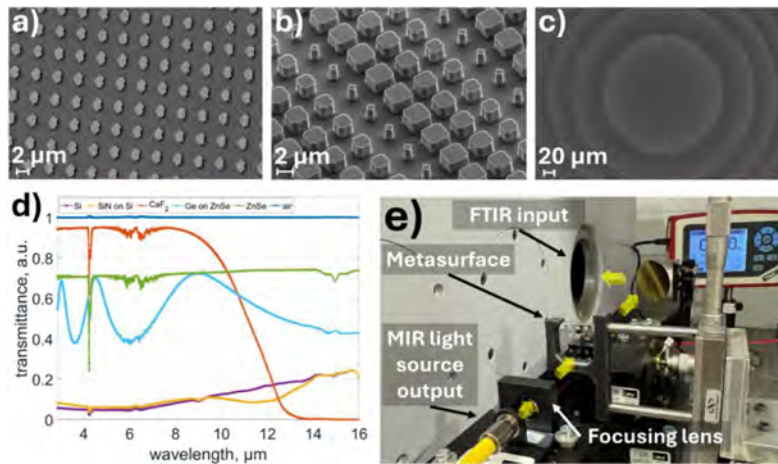
2. Tyndall National Institute, T12 PX46, Cork, Ireland

3. Institute of Chemical Technologies and Analytics, TU Wien, Getreidemarkt 9/164, Vienna, 1060, Austria

4. Department of Electrical and Information Engineering, Politecnico di Bari, Via E. Orabona, 4, 70126 Bari, Italy

**Short abstract:** This work reviews metamaterials, such as metasurfaces, metadeflectors and metalenses application in the field of spectroscopy covering the mid-IR range. Their possible application with focus on the fabrication and experimental characterization approaches are discussed.

Metamaterials are artificially engineered surfaces or a planar 2D nanostructures that aim to control the propagation of electromagnetic waves [1]. The unique ability of metamaterials to manipulate light has led to their exploration in various applications, including: metaabsorbers [2], metalenses and metareflectors [3], metasurfaces for spectroscopy [4], [5] and chiral metasurfaces for biosensing applications [1]. Examples of the metastructures are presented in the Figures 1 (a)-(c).



**Fig. 1** SEM images of the part of: a) metasurface, b) metadeflector and c) metalens. d) FTIR spectra of the materials used in fabrication processes. e) FTIR-based metasurfaces characterisation setup

In this work we overview the metasurfaces application for the infrared spectroscopy paying attention to the fabrication process requirements. The materials absorption in the wide range of the Mid-IR wavelength forces the fabrication platform selection for each particular cases. In this regard the Si/Si<sub>3</sub>N<sub>4</sub>/CaF<sub>2</sub> platforms covers the wavelength range up to ~6/9/8 μm respectively and ZnSe/Ge platform covers further ranges up to 15 μm (see Figure 1d).

Additional difficulties are caused by the fabrication techniques choice. The required feature sizes for the beam manipulating are tending to be small (< 1 μm) but at the same time the whole device dimensions are much bigger and dictated by the beam spot size (> 1 mm, see Figure 1e). This makes E-Beam lithography unsuitable due to the high-cost and with photolithography 1 μm feature size (contact) and 0.5 μm (stepper) are close to the limits for what is required.

Fabricated germanium-based metamaterials will be used for the Mid-IR light delivery system for the QEPAS. The silicon-based metamaterials will next be used for the surface enhanced IR absorption spectroscopy and Photothermal spectroscopy

**Acknowledgements:** E.U. Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 860808 (OPTAPHI), the EVOQUE Project Grant Agreement No 101135764, and the MetaSPECS Project funded by the Science Foundation Ireland (SFI) 21/FFP-A/10002.

## References

- [1] S. Roy, S. Mondal, and K. Debnath, "Graphene-Based Chiral Metasurface for Generation of Tunable Circular Dichroism—Design and Sensor Applications," *IEEE Sens. J.*, vol. 23, no. 1, pp. 285–292, Jan. 2023, doi: 10.1109/JSEN.2022.3221437.
- [2] S. Roy and K. Debnath, "Graphene-based electromechanically tunable subwavelength mid-IR perfect absorber," *Opt. Quantum Electron.*, vol. 55, no. 14, p. 1246, Dec. 2023, doi: 10.1007/s11082-023-05514-0.
- [3] A. Arbabi, R. M. Briggs, Y. Horie, M. Bagheri, and A. Faraon, "Efficient dielectric metasurface collimating lenses for mid-infrared quantum cascade lasers," *Opt. Express*, vol. 23, no. 26, p. 33310, Dec. 2015, doi: 10.1364/OE.23.033310.
- [4] K. Koshelev and Y. Kivshar, "Dielectric Resonant Metaphotonics," *ACS Photonics*, vol. 8, no. 1, pp. 102–112, Jan. 2021, doi: 10.1021/acsp Photonics.0c01315.
- [5] G. Piscopo, A. S. Vorobev, G. Magno, and L. O'Faolain, "High-FoM All-Dielectric Metasurface for Advanced Mid-IR Sensing Applications," in *2024 IEEE International Humanitarian Technologies Conference (IHTC)*, Bari, Italy: IEEE, Nov. 2024, pp. 1–6. doi: 10.1109/IHTC61819.2024.10855116.

# Mid-IR Spatial Light Modulation Using Germanium Metamaterials

J. H. Mendoza-Castro<sup>1,2\*</sup>, G. Piscopo<sup>2,3</sup>, A. S. Vorobev<sup>3,4</sup>, T. Piwonski<sup>4</sup>, A. D’Orazio<sup>2</sup>,  
G. Magno<sup>2</sup>, B. Lendl<sup>1</sup> and L. O’Faolain<sup>3,4</sup>

1. Institute of Chemical Technologies and Analytics, TU Wien, Getreidemarkt 9/164, Vienna, 1060, Austria.

2. Department of Electrical and Information Engineering, Politecnico di Bari, Via E. Orabona, 4, 70126 Bari, Italy

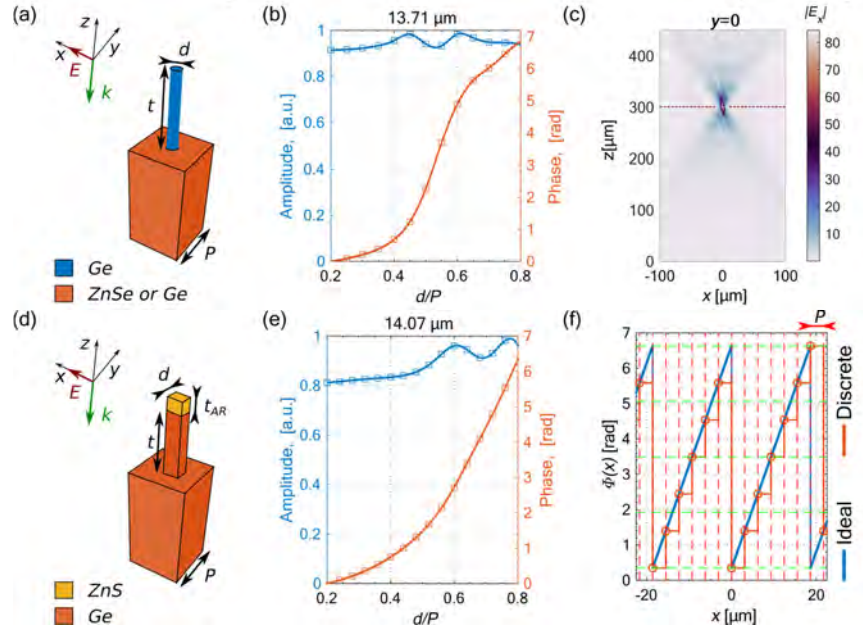
3. Centre for Advanced Photonics and Process Analysis, Munster Technological University, T12 T66T, Cork, Ireland

4. Tyndall National Institute, T12 PX46 Cork, Ireland

\*corresponding author: [jesus.mendoza-castro@tuwien.ac.at](mailto:jesus.mendoza-castro@tuwien.ac.at)

**Short abstract:** We present the numerical design and characterization of Germanium-based metamaterials for long-wavelength infrared (LWIR, 12–15  $\mu\text{m}$ ) applications. These structures enable field enhancement, broadband high reflectivity, beam steering, focusing, and collimation, addressing the growing demand for compact and efficient optical components in the LWIR range.

Volatile organic compounds (VOCs) exhibit strong absorption in the LWIR range, enabling highly selective detection [1]. While photothermal and photoacoustic spectroscopy offer high sensitivity, miniaturization remains challenging due to the limited availability of compact mid-IR components. LWIR metalenses [2] present a promising solution, enabling compact, high-performance optical elements. This work explores Germanium-based engineered meta-optics for field enhancement, broadband high reflectivity, beam steering, focusing, and collimation, aligned with VOC absorption bands, to advance miniaturized LWIR sensing technologies.



**Fig. 1** Design and simulation of Germanium-based metamaterials for LWIR applications. (a) Ge unit cell on a ZnSe substrate or bulk Ge. (b) Simulated amplitude and phase response as a function of the filling fraction ( $d/P$ ). (c) Cross-section of the simulated diffracted beam along the z-axis for a metalens with a 300  $\mu\text{m}$  focal length, 700  $\mu\text{m}$  diameter, and  $NA = 0.8$ . (d) Bulk Ge meta-atom with ZnS anti-reflection coating. (e) Simulated amplitude and phase response as a function of  $d/P$ . (f) Ideal and discrete phase distribution  $\Phi(x)$  of a meta-deflector designed for  $\sim 10^\circ$  beam deflection.

Rigorous Coupled Wave Analysis is employed to compute the amplitude and phase response of the proposed meta-atoms, Fig. 1(a & d). As shown in Fig. 1(b & e), all cases achieve a full  $2\pi$  phase coverage while maintaining transmission above 75%. These meta-atoms enable the design of high-NA metalenses, meta-deflectors, and other structures. Fig. 1(c) illustrates the spatial amplitude field distribution along the propagation axis, while Fig. 1(f) presents the ideal and discrete spatial phase distributions along the transverse axis. These phase-front manipulations contribute to a set of devices designed to enhance spectroscopy systems in the LWIR range.

**Acknowledgments:** E.U. Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 860808 (OPTAPHI), and the EVOQUE Project Grant Agreement No 101135764.

## References

- [1] Kinjalk, K. et al., “Highly selective and sensitive detection of volatile organic compounds using long wavelength InAs-based quantum cascade lasers through quartz-enhanced photoacoustic spectroscopy,” *Applied Physics Reviews*, vol. 11, no. 2, p. 021427, 2024,
- [2] Nalbant, H. C. et al., “Transmission optimized LWIR metalens,” *Appl. Opt.*, AO, vol. 61, no. 33, pp. 9946–9950, 2022,
- [3] Kotlyar, V. V. et al., “Thin High Numerical Aperture Metalens,” *Opt. Express*, Vol. 25, No. 7, 8158–8167, 2017.
- [4] Mendoza-Castro, J. et al., “Metasurface-Enhanced Mid-Infrared Sensing Based on Integrated Polycrystalline Silicon Metagratings,” *IEEE IHTC*, 1–6, 2024.



# Novel Infrared Sources and Detectors



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# Shaping Photon Statistics in Mid-Infrared Cascade Lasers

Irene La Penna<sup>1</sup>, Tecla Gabbriellini<sup>1,2</sup>, Borislav Hinkov<sup>3</sup>, Robert Weih<sup>4</sup>, Naota Akikusa,<sup>5</sup> Simone Borri<sup>1,2</sup>, Luigi Consolino<sup>1,2</sup>, Alessio Montori<sup>1,6</sup>, Lorenzo Mischì<sup>6</sup>, Francesco Cappelli<sup>1,2</sup>, Paolo De Natale<sup>1,2</sup>

1. LENS - European Laboratory for Non-Linear Spectroscopy, Via Carrara, 1 - 50019 Sesto Fiorentino FI, Italy

2. CNR-INO - Istituto Nazionale di Ottica, Largo Fermi, 6 - 50125 Firenze FI, Italy

3. Silicon Austria Labs, Europastraße 12, 9524 Villach, Austria

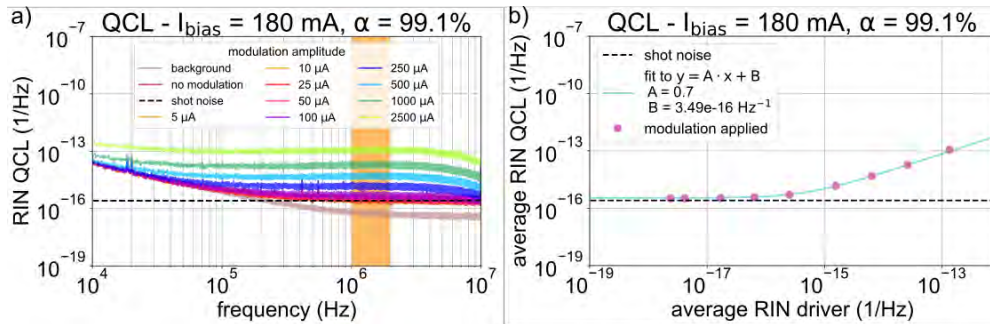
4. Nanoplus Nanosystems and Technologies GmbH - Gleimershäuser Strasse 10, 98617 Meiningen, Germany

5. SSD advanced innovation headquarters, Hamamatsu Photonics K.K., Shizuoka 431-2103, Japan

6. ppqSense Srl, V.le L. Ariosto, 492B, 50019 Sesto Fiorentino FI, Italy

**Short abstract:** We study how the current noise is transferred to photon emission in Quantum and Interband Cascade Lasers. In particular, we investigate how supplying current with a noise below the shot-noise classical limit affects laser emission, in terms of laser intensity noise.

Reducing the intensity noise of coherent light sources is of utmost interest for a variety of applications, ranging, e.g., from metrology to spectroscopy. In our group, we pioneered a full understanding of the physical mechanisms underpinning observed frequency noise in QCLs [1,2] and ICLs [3], unveiling the intrinsic laser linewidth in these lasers. More recently, we focused the attention on intensity noise in these two classes of lasers, trying to understand, even using ultracold atoms as quantum simulators of electron transport in quantum wells [4], if sub-classical effects could be observed in the photon emission [5-7]. Intensity noise squeezing in bipolar semiconductor lasers was observed by Yamamoto et al. [8], by feeding the laser with current from a low-noise driver. In our experiments, we use two mid-IR emitting lasers, a QCL and an ICL, fed by a driver (from ppqSense Srl) built to generate current exhibiting an intensity noise more than 10 dB below the shot noise, in the best conditions. In these conditions we could measure the transfer function from electric bias current fluctuations to emitted intensity fluctuations. To this aim, the lasers were driven using a low-noise bias current, as described above, modulated by a white noise of varying amplitude. The emitted light, after proper attenuation, is collected onto a detector and the relative intensity noise (RIN) of the two lasers is measured via a spectrum analyzer. We acquire RIN spectra for different values of white noise amplitude and average them in a suitable frequency range, as represented by the orange area in Fig. 1(a). The average laser RIN is plotted against the RIN of the current driver measured at the corresponding modulation amplitude (Fig 1(b)), thus mapping the laser intensity noise fluctuations onto the laser fluctuations of the bias current. The retrieved transfer function is a linear expression, whose slope is defined as the transfer coefficient and characterizes the transfer of noise from the current driver to the laser.



**Fig. 1** (a) RIN spectra of the QCL driven at 180 mA of bias current with optical attenuation  $\alpha$  of 99.1%, for different values of white noise amplitude, as reported in the legend. The black dashed line is the calculated laser shot noise, the old-rose trace is the detector thermal background, and the orange shaded area indicates the frequency range where the spectra were averaged. (b) Average RIN plotted against the current driver RIN for the corresponding values of modulation amplitude. The function relating the two is the transfer function between bias current fluctuations and laser intensity fluctuations.

The about 99% attenuation of the laser power, that is necessary to match the limited dynamic range of the available detectors, actually cancels possible sub-classical effects and gives back shot noise-limited radiation. In conclusion, this work proposes a way to characterize and quantify the transfer of noise from the electrical bias current to the photon statistics of a laser. The results obtained for the two tested lasers show that classical noise can be actively transferred from electrons to photons. Choosing IR detectors with a higher dynamic range could focus the attention onto the quantum efficiency and shed light on the internal physics of the lasers. In turn, this will help to redesign cascade lasers, in view of higher emission efficiency and new performance for Quantum Technologies.

## References

- [1] S. Bartalini, et al., “Observing the Intrinsic Linewidth of a Quantum-Cascade Laser: Beyond the Schawlow-Townes Limit”, *Phys. Rev. Lett.* **104**, 083904 (2010).
- [2] M.S. Vitiello, et al., “Quantum-limited frequency fluctuations in a terahertz laser”, *Nat. Photonics* **6**, 525 (2012).
- [3] S. Borri, et al., “Unveiling quantum-limited operation of interband cascade lasers”, *APL Photonics* **5**, 036101 (2020).
- [4] A. Trombettoni, et al., “Quantum Simulating the Electron Transport in Quantum Cascade Laser Structures”, *Adv. Quantum Technol.* **4**, 2100044 (2021).
- [5] T. Gabbrielli, et al., “Mid-infrared homodyne balanced detector for quantum light characterization,” *Opt. Express* **29** (2021).
- [6] T. Gabbrielli, et al., “Intensity correlations in quantum cascade laser harmonic frequency combs,” *Adv. Photonics Res.* **3** (2022).
- [7] T. Gabbrielli, J. Pelini, et al., “Shot-noise-limited emission from interband and quantum cascade lasers,” *arXiv preprint arXiv:2409.12732* (2024).
- [8] Y. Yamamoto, S. Machida, and O. Nilsson, “Amplitude squeezing in a pump-noise-suppressed laser oscillator,” *Phys. Rev. A* **34** (1986)



# Laser-textured Quartz-Tuning-Forks for Light-Induced Thermoelastic Spectroscopy

Raffaele De Palo<sup>1</sup>, Annalisa Volpe<sup>1,2</sup>, Pietro Patimisco<sup>1,3</sup>, Andrea Zifarelli<sup>1</sup>, Angelo Sampaolo<sup>1,3</sup>, Antonio Ancona<sup>1,2</sup>, Vincenzo Spagnolo<sup>1,3</sup>

1. Dipartimento Interateneo di Fisica, Politecnico of Bari & Università degli Studi di Bari, Via G. Amendola 173, Bari 70125, Italy

2. CNR-IFN UOS BARI, Via Amendola 173, Bari, Italy

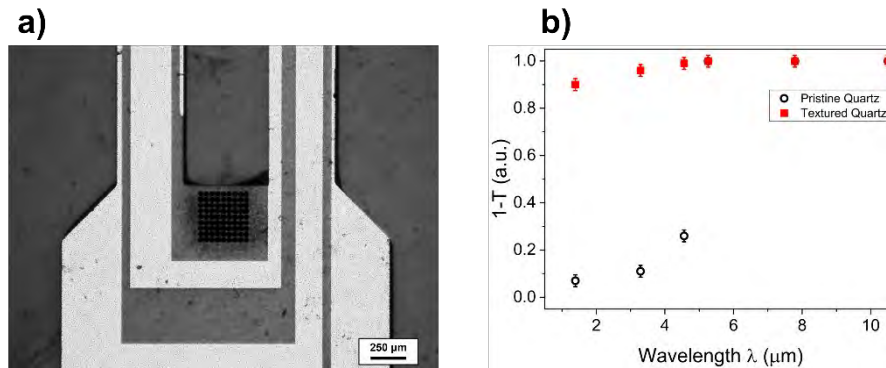
3. PolySense Innovations srl, Via Amendola 173, Bari 70126, Italy

**Short Abstract:** Light-Induced Thermoelastic-Spectroscopy exploits Quartz-Tuning-Forks as photodetectors for gas sensing. This approach is limited to wavelengths longer than 5  $\mu\text{m}$  since below this threshold quartz is transparent. This issue has been addressed using a femtosecond pulsed laser to enhance absorption of Quartz-Tuning-Forks for  $\lambda < 5 \mu\text{m}$  through superficial texturing.

Quartz-Tuning-Forks (QTFs) have been widely and successfully exploited as acoustic detectors in Quartz-Enhanced-Photoacoustic-Spectroscopy (QEPAS) and as photodetector in Light-Induced-Thermoelastic Spectroscopy (LITES) [1]. In LITES, an intensity-modulated laser beam resonant with a radiative transition of the target gas, is focused on the QTF surface. The portion of light absorbed by the QTF creates a local heat accumulation: the increase of the local temperature generates nearby a strain field proportional to the thermal expansion coefficient of quartz. As a result, this opto-thermo-elastic conversion produces an electrical signal proportional to the absorbed light intensity because of the quartz piezoelectricity. The main limitation to this technique is related to the absorption spectrum of quartz: this material is almost transparent ( $T > 95\%$ ) for wavelengths below 5  $\mu\text{m}$ , thus limiting the detection band of the device in the Mid-Infrared (MIR).

This issue has been addressed through superficial texturing of the quartz surface using a femtosecond pulsed laser, thereby extending its optical absorption into the Near-Infrared (NIR) wavelength range. This approach has been already used in the past for enhancing the optical absorption of different materials such, silicon [2] and diamond [3].

In Fig. 1, an image of a laser textured QTF is shown together with its measured  $I$ - $T$  spectrum compared to the spectrum of pristine quartz in the 1-10  $\mu\text{m}$  wavelength range.



**Fig. 1** Laser textured QTF (a) together with its  $I$ - $T$  plot compared with that of pristine quartz (b).

The texturing has been realized as a square matrix of ablated craters on the QTF surface, as shown in Fig. 1(a). The plot in Fig. 1(b) shows that the texturing does not affect the absorbance of the quartz crystal in the opaque region, which consistently remains above 98%. Conversely, superficial texturing significantly enhances the absorbance in the transparent region. The QTF was thus integrated into a LITES setup to detect a water absorption feature at 1.39  $\mu\text{m}$ , achieving a responsivity of  $R = 14.6 \mu\text{AW}^{-1}$ . It was also employed to detect another water absorption feature at 7.38  $\mu\text{m}$ , yielding a comparable responsivity of  $R = 17 \mu\text{AW}^{-1}$ .

These findings highlight the potential of laser textured quartz for broadband infrared photodetection.

## References

- [1] A. Zifarelli, R. De Palo, S. Venck, F. Joulain, S. Cozic, R. Weih, A. Sampaolo, P. Patimisco, V. Spagnolo, "Methane and ethane detection from natural gas level down to trace concentrations using a compact mid-IR sensor based on light-induced thermoelastic spectroscopy and univariate calibration," *Photoacoustics*, vol. 29, p. 100448, Jan. 2023, doi: 10.1016/J.PACS.2023.100448.
- [2] A. Y. Vorobyev and C. Guo, "Direct creation of black silicon using femtosecond laser pulses," *Appl. Surf. Sci.*, vol. 257, no. 16, pp. 7291–7294, Jun. 2011, doi: 10.1016/j.apsusc.2011.03.106.
- [3] P. Calvani, A. Bellucci, M. Girolami, S. Orlando, V. Valentini, R. Polini, D. M. Trucchi, "Black diamond for solar energy conversion," *Carbon N. Y.*, vol. 105, pp. 401–407, Aug. 2016, doi: 10.1016/J.CARBON.2016.04.017.

# Lithium Niobate Tuning Forks as piezoelectric transducers in Infrared Spectroscopy for gas sensing

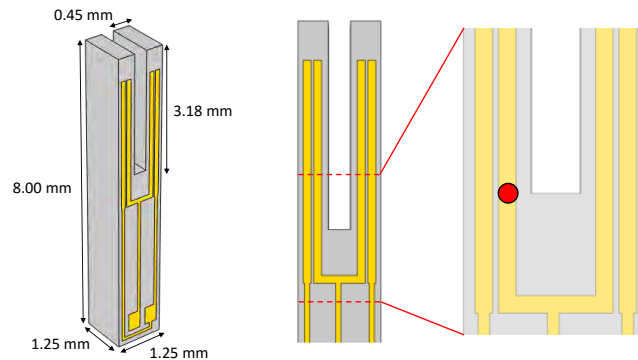
Aldo F. P. Cantatore<sup>1</sup>, Giansergio Menduni<sup>1,2</sup>, Andrea Zifarelli<sup>1,2</sup>, Pietro Patimisco<sup>1,2</sup>, Vincenzo Spagnolo<sup>1,2</sup>, Angelo Sampaolo<sup>1,2</sup>

1. Polysense Lab, University and Polytechnic of Bari, Via G. Amendola, 173, 70126, Bari – Italy

2. Polysense Innovations srl, Via G. Amendola, 173, 70126, Bari – Italy

**Short abstract:** Lithium niobate has emerged as a highly sought after material for integrated photonics applications. The operation of a lithium niobate tuning fork as a piezoelectric transducer in photoacoustic spectroscopy and tunable diode laser absorption spectroscopy is reported, thus paving the way for all-integrated on-chip sensing platforms.

Lithium niobate (LiN) has emerged as one of the most extensively used materials in integrated photonics over the past two decades, owing to its remarkable electro-optic, acousto-optic, and nonlinear optical properties. In addition, its physical and chemical stability, wide transparency range (0.4–5  $\mu\text{m}$ ), as well as its high refractive index make it a highly desirable material for such applications. Furthermore, LiN has been extensively deployed in the development of piezoelectric devices, such as tuning forks (TFs), thanks to its high electromechanical coupling coefficient [1]. In this work, we report on the employment of a lithium niobate tuning fork (LiNTF) prototype as a piezoelectric transducer in infrared spectroscopy applications devoted to gas sensing. The LiNTF (depicted in Fig. 1a), fabricated from a 128° Y-cut LiN wafer and showing a fundamental resonance frequency of 40.63 kHz, was first employed as an acoustic wave detector in a photoacoustic (PAS) point sensor. The detection of water vapor, targeting the absorption feature located at 7181.15  $\text{cm}^{-1}$ , shows comparable performances to a standard 32 kHz – quartz tuning fork (QTF) employed in the same PAS setup [2]. The same LiNTF was employed as an infrared photodetector in tunable diode laser absorption spectroscopy (TDLAS). As already demonstrated over the last few years for QTFs [3], the thermoelastic conversion of optical energy in piezoelectric transducers allows the detection of modulated infrared laser light. Indeed, the absorbed optical power in the device will generate a local strain field, leading in turn to a measurable electric signal owing to LiN or quartz piezoelectricity. In the reported TDLAS experiment, the same laser source for the PAS detection of water vapor was employed and the optical power was focused on the rear surface of the resonator, where no gold electrodes are deposited (Fig. 1b).



**Fig. 1** a) Sketch of the LiNTF prototype geometry showing the deposition pattern of the gold electrodes; b) Detail of the LiNTF front and rear surfaces showing the laser focusing point (red dot) adopted to carry out TDLAS measurements.

Even though LiN is transparent to the selected laser wavelength (1.39  $\mu\text{m}$ ), light is extinguished by the chromium layer used as a primer to let the gold pads adhere to the resonator surface. Compared to a 9.8 kHz – QTF, showing the best responsivity as an infrared photodetector [3], the LiNTF demonstrated a twice worse detection sensitivity, though showing a higher stability as a result of an Allan-Werle deviation analysis. Nevertheless, the LiNTF performance as an infrared photodetector could be further improved by optimizing its geometry and gold pad deposition pattern to increase its active area, as well as by doping the LiN crystal or depositing thin films on the resonator surface to enhance its absorbance.

## References

- [1] M. González, G. Ham, A. Al Haddad, G. Bernero, and M. Deffenbaugh, “Downhole viscosity measurement platform using tuning fork oscillators”, *2015 IEEE SENSORS*, 1-4 (2015).
- [2] A.F.P. Cantatore, G. Menduni, A. Zifarelli, P. Patimisco, M. Gonzalez, H.R. Seren, V. Spagnolo, and A. Sampaolo, “Lithium Niobate – Enhanced Photoacoustic Spectroscopy”, *Photoacoustics* **35**, 100577, (2024).
- [3] T. Wei, A. Zifarelli, S. Dello Russo, H. Wu, G. Menduni, P. Patimisco, A. Sampaolo, V. Spagnolo, and L. Dong, “High and flat spectral responsivity of quartz tuning fork used as infrared photodetector in tunable diode laser spectroscopy”, *Appl. Phys. Rev.* **8**, 041409 (2021).

# Ge-on-Si bias-tunable dual-band photodetector for solvent recognition

Afonso de Cerdeira Oliveira <sup>1</sup>, Andrea Barzaghi <sup>1</sup>, Raffaele Giani <sup>1</sup>, Jacopo Frigerio <sup>1</sup>, Andrea De Iacovo <sup>2</sup>  
Lorenzo Colace <sup>2</sup>, Andrea Ballabio <sup>1</sup>, Giovanni Isella <sup>1</sup>

1. L-NESS Dipartimento di Fisica, Politecnico di Milano, 22100 Como, Italy

2. Dipartimento di Ingegneria Industriale, Elettronica e Meccanica, Università Roma Tre, 00146, Roma, Italy

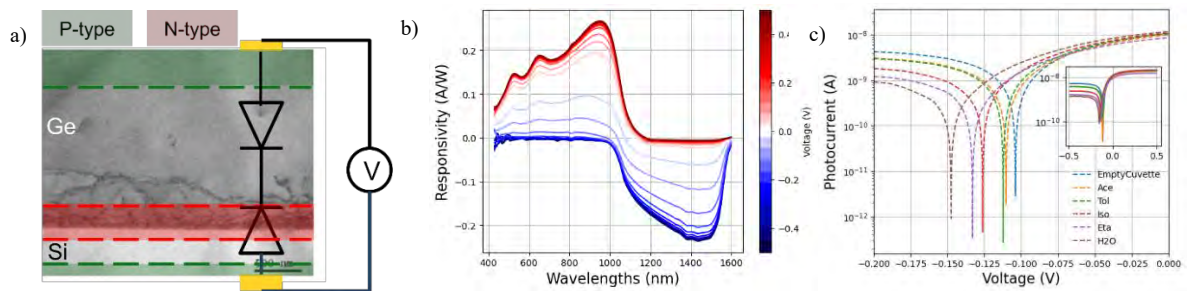
**Short abstract:** CMOS-compatible Ge-on-Si dual-band detectors in back-to-back architecture can fine-tune their spectral responsivity through small voltage-bias control, enabling them to collect and combine data, at pixel level and under similar light conditions, from visible to infrared, retrieving information that neither band can provide by itself, contributing with important advances for imaging.

Light sensing beyond the visible spectra has always played an important role in scientific advances. The possibility to acquire and combine information from visible (VIS) and infrared (IR) ranges, exploiting IR optical windows and reduced Rayleigh scattering can lead to key-point advances in recognition systems, environmental sensing, failure analysis, or even in emerging applications such as cameras for advanced driver assistance systems [1]. By connecting two photodiodes in a back-to-back configuration [see Fig. 1a], it is possible to sense different spectral ranges depending on the semiconductors bandgap and applied voltage [2]. Resorting on germanium (Ge) and silicon (Si), it is possible to cover the short-wave infrared (SWIR) ( $\lambda = 800 - 1600$ ) and VIS, and near infrared (NIR), ( $\lambda = 400 - 1100$ ), respectively, where the device responsivity can be tuned by controlling the voltage-bias magnitude and polarity [see Fig. 1b)]. In such a way bias-scans acquire data at pixel level and under similar illumination conditions, enabling reliable information combination to accomplish enhanced applications. The open circuit voltage ( $V_{oc}$ ) that occurs when photocurrent goes to zero ( $I_{ph} = 0$ ) depends on a thermal voltage  $V_T$ , and the natural logarithm of the ratio between the photo and dark currents of the individual photodetectors.

$$V_{oc} = V_T \ln \left( \frac{I_{ph}^{Ge} I_0^{Si}}{I_{ph}^{Si} I_0^{Ge}} \right)$$

Displacements on  $V_{oc}$  are dominated by variations on  $I_{ph}^{Ge}/I_{ph}^{Si}$  [3], feature exploited to discriminate between transparent solvents in VIS but with distinct absorption in IR, enabling solutions discrimination by  $V_{oc}$  displacements of a few mV [See Fig1. c)]. Furthermore, the light source spectra can be adequately refined, highlighting spectral regions where compounds under test present higher IR absorption differences, enhancing displacements in  $V_{oc}$  since the photocurrent is directly dependent on the impinging light power density. Additionally, the Ge-on-Si compatibility with CMOS processes allows compact, reliable and scalable detectors that can be produced at low cost and operate at low voltage bias.

In summary, we demonstrate a compact and scalable dual-band detector in a back-to-back architecture, operating from visible to SWIR able to discriminate between different substances without any mechanical or dispersive element, reducing the necessity of complex optical assemblies to cover broad light spectra or the need of several detectors.



**Fig. 1** (a) Schematic representation of the dual-band detector (b) Device responsivity measured for several voltage bias (c) photocurrent-voltage curves for the different solvents in measure.

## References

- [1] Swaminathan, K., et al. "Optically-aligned visible/near-infrared dual-band photodetector materials and devices on GaAs using metamorphic epitaxy." *Journal of Applied Physics* 110.6 (2011): 063109
- [2] Simola, E. T.; De Iacovo, A.; Frigerio, J.; Ballabio, A.; Fabbri, A.; Isella, G.; Colace, L. Voltage-tunable dual-band Ge/Si photodetector operating in VIS and NIR spectral range. *Optics express* 2019, 27, 8529–8539
- [3] Nouchi, R. Extraction of the Schottky parameters in metalsemiconductor-metal diodes from a single current-voltage measurement. *Journal of Applied Physics* 2014, 116, 184505



# New capacitive MEMS design for photoacoustic gas sensing

Fanny Pages<sup>1</sup>, Julien Charensol<sup>1</sup>, Julie Goutorbe<sup>1</sup>, Tarek Seoudi<sup>1</sup>, Diba Ayache<sup>1</sup>, Eric Rosenkrantz<sup>1</sup>,  
Aurore Vicet<sup>1</sup>, Michael Bahriz<sup>1</sup>

*1. Institut d'Electronique et des Systèmes - University of Montpellier - 34090 Montpellier (France)*

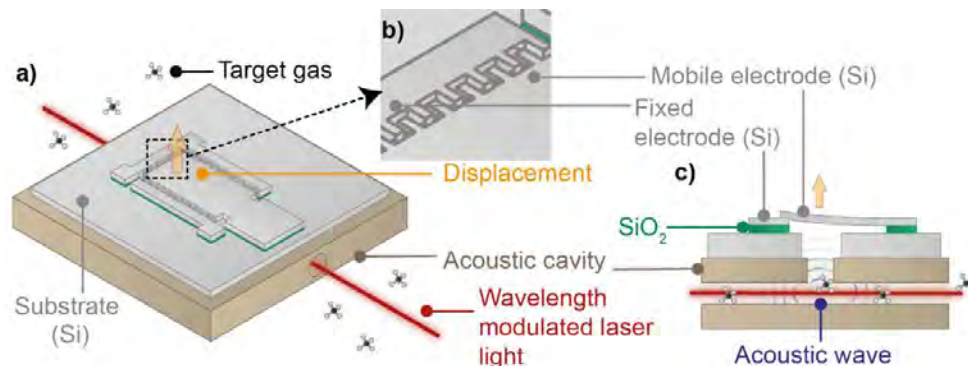
**Short abstract:** A new silicon-based capacitive sensor has been developed for photoacoustic gas detection, optimizing photoacoustic wave collection and minimizing viscous damping. This new design has successfully improved by a factor 2 the sensor's limit of detection compared to our previous design. Ongoing work aims to further improve this performance.

Photoacoustic spectroscopy (PAS) offers a promising approach for developing compact, cost-effective, and highly sensitive trace gas sensors. Indeed, this technique is independent of the optical path, enabling operation with very small volumes of gas and real-time measurements. Building on these advantages, our integrated MEMS[1] represents a unique PAS implementation, specifically designed to optimize photoacoustic wave collection while maintaining high nominal capacitance and minimizing viscous damping[2].

The MEMS device, referred to as Centipede and shown in Figure 1.a) and b), consists of a cantilever dedicated to photoacoustic energy harvesting, surrounded by interdigitated arms dedicated to capacitive transduction by surface variation. A hole below the cantilever prevent the gas from being trapped and compressed between closely spaced surfaces (squeeze film damping). This design is then coupled to an acoustic cavity, shown in Figure 1.c), with the same resonant frequency as the MEMS to increase the pressure applied to the MEMS. The use of an acoustic cavity is crucial to enhance the acoustic force and minimise potential photothermal noise, thereby improving the signal-to-noise ratio (SNR). The acoustic cavity dimensions were optimized using COMSOL Multiphysics simulations.

Allan-Werle deviation analysis revealed that the MEMS device achieved, for methane, a limit of detection (LOD) of 52 ppmv with one second integration time for first harmonic detection leading to a Normalised Noise Equivalent Absorption Coefficient (NNEA) of  $4.17 \cdot 10^{-8} \text{ cm}^{-1} \cdot \text{W}/\sqrt{\text{Hz}}$  for the MEMS device.

This new design eliminates the major issue of our previous designs while improving by a factor 2 the sensor's limit of detection[3]. However, suppressing the squeeze film effects also introduces the Couette effect, which plays a major role in enhancing the quality factor of the MEMS. Therefore, despite its NNEA of  $4.17 \cdot 10^{-8} \text{ cm}^{-1} \cdot \text{W}/\sqrt{\text{Hz}}$ , our MEMS still has room for improvement as it is our first result. Our goal is to further enhance the sensor's performance. We are currently developing a new design with a lower effective mass and greater efficiency, while also exploring improvements to the manufacturing process.



**Fig. 1** a) Illustration of Centipede resonator. The resonator is divided in two parts: a cantilever, movable, is dedicated for photoacoustic energy collection, and electrodes, fixed, are dedicated to the surface variation capacitive transduction. b) A detailed view of the electrodes. c) Schematic illustration of an acoustic cavity placed under the MEMS. The length of the cavity  $L_{mR}$  depends on the resonant frequency targeted. Here  $L_{mR} = 14.5 \text{ mm}$  and its resonant frequency  $f_0 = 14.4 \text{ kHz}$ .

## References

- [1] K. Chamassi, W. Trzpil, R. Arinero, R. Rousseau, A. Vicet, and M. Bahriz, "Capacitive silicon micro-electromechanical resonator for enhanced photoacoustic spectroscopy", *Appl. Phys. Lett.* **115**, 081106 (2019).
- [2] W. Trzpil, N. Maurin, R. Rousseau, D. Ayache, A. Vicet, and M. Bahriz, "Analytic optimization of cantilevers for photoacoustic gas sensor with capacitive transduction", *Sensors* **21**, 1489 (2021).
- [3] T. Seoudi, J. Charensol, W. Trzpil, F. Pages, D. Ayache, R. Rousseau, A. Vicet, and M. Bahriz, "Highly Sensitive Capacitive MEMS for Photoacoustic Gas Trace Detection", *Sensors* **23**, 3280 (2023).

# Exploiting unconventional silicon-based Micro-Electro-Mechanical systems for high-sensitivity cantilever-enhanced photoacoustic spectroscopy

Jacopo Pelini<sup>1</sup>, Stefano Dello Russo<sup>2</sup>, Mario Siciliani de Cumis<sup>2</sup>, Iacopo Galli<sup>1</sup>, Pablo Cancio Pastor<sup>1</sup>, Zhen Wang<sup>4</sup>, Maria Concetta Canino<sup>3</sup>, Alberto Roncaglia<sup>3</sup>, Wei Ren<sup>4</sup>, Paolo De Natale<sup>1</sup>, and Simone Borri<sup>1</sup>

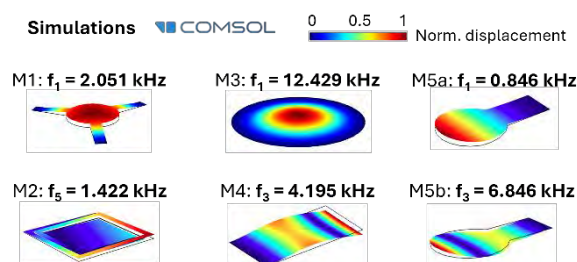
1. CNR-INO - Istituto Nazionale di Ottica, Largo E. Fermi 6, 50125 Firenze, and LENS, via N. Carrara 1, 500192.
2. ASI Agenzia Spaziale Italiana - Centro di Geodesia Spaziale, Località Terlecchia, 75100, Matera, Italy.
3. Istituto per la Microelettronica e Microsistemi (IMM), Consiglio Nazionale delle Ricerche (CNR), Via P. Gobetti 101, 40129 Bologna, Italy.
4. Department of Mechanical and Automation Engineering, The Chinese University of Hong Kong, New Territories, Hong Kong SAR, China.

**Short abstract:** Leveraging on Micro Electro Mechanical System (MEMS) technology, we explore unconventional silicon-based acoustic transducers with alternative geometries to the standard rectangular shape. These structures, optimized through simulations and experiments, demonstrate flexibility across various resonance frequencies and optimal pressure conditions, allowing to cover different trace-gas detection applications.

Driven by the increasingly scientific effort and technological innovation, trace-gas sensing has become deeply interconnected with our daily life, finding applications in a lot of sectors. Among all it is worth mentioning as examples the field of environmental monitoring, breath analysis, and industrial process control. During the last two decades photoacoustic spectroscopy (PAS) has emerged as powerful tool for highly sensitive trace-gas detection, offering a valid alternative to conventional direct-absorption approaches. In a photoacoustic-based setup, the target gas under examination selectively absorbs a modulated laser light and generates acoustic waves by non-radiative relaxation processes. Exploiting a proper acoustic transducer is then possible to convert the acoustic waves into a measurable signal, also defined as photoacoustic signal.

Based on this consideration, this technique can count on important advantages. Firstly, being an indirect detection approach, no photo-detectors are needed to measure the molecule's absorption spectrum, thus determining an high level of scalability and tunability. Secondly, this technique offers a high degree of flexibility, since the maximization of the detection performance can be obtained by simultaneously playing with the key experimental components [1]. In this sense, a crucial role is played by the acoustic transduction part.

Taking advantage of the possibility offered by Micro-Electro-Mechanical systems (MEMS), we proposed and investigated novel and unconventional geometries of silicon-based acoustic transducers for trace-gas detection, overcoming the standard rectangular shape [2]. Starting from *ab initio* simulations of their resonance frequencies via Finite Element Modelling (FEM), their mechanical properties and photoacoustic responses have been experimentally tested in a conventional PAS-based setup.



**Fig. 1** An example of the silicon-based MEMS investigated, associated with the resonance mode analysed.

Given the wide range of resonance frequencies investigated (within 0.8 and 12.5 kHz), our structures have proven to be excellent candidates for high-performing trace-gas sensors, addressing also different optimal sample pressure conditions. In particular, MEMS structures at higher resonance frequencies showed the potentiality of achieving high detection sensitivity level by the combination with optical and acoustic resonances [3,4]. On the other side, MEMS structure with lower resonance frequencies have been exploited for fundamental studies, comparing the performances of amplitude (1f) and wavelength (2f) modulation PAS-based detection.

## References

- [1] Patimisco, Pietro, et al. "Quartz-enhanced photoacoustic spectroscopy: a review." *Sensors* 14.4 (2014): 6165-6206;
- [2] Pelini, Jacopo, et al. "New silicon-based micro-electro-mechanical systems for photo-acoustic trace-gas detection." *Photoacoustics* 38 (2024): 100619;
- [3] Russo, Stefano Dello, et al. "Dual-tube MEMS-based spectrophone for sub-ppb mid-IR photoacoustic gas detection." *Photoacoustics* 40 (2024): 100644;
- [4] Pelini, Jacopo, et al. "A cavity-enhanced MEMS-based photoacoustic sensor for ppt-level trace-gas detection." *Sensors and Actuators B: Chemical* (2025): 137313.

# Optical Sensing and Spectroscopy



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# Spectroscopic applications of novel ultra-broadband, mid-infrared IDFG-based sources

Roderik Krebbers<sup>1</sup>, Amir Khodabakhsh<sup>1,2</sup>, Simona M. Cristescu<sup>1</sup>

1. Life Science Trace Detection Laboratory, IMM, Radboud University, 6525 AJ Nijmegen, The Netherlands

2. Circular Chemical Engineering, Faculty of Science and Engineering, Maastricht University, 6229 GS Maastricht, The Netherlands

**Short abstract:** Novel intrapulse difference-frequency generation (IDFG)-based laser systems possess a unique combination of high power output, coherence, low noise and broad spectral mid-infrared coverage. We demonstrate multi-species gas sensing applications with this source, ranging from environmental sensing with open-path spectroscopy to exhaled breath analysis.

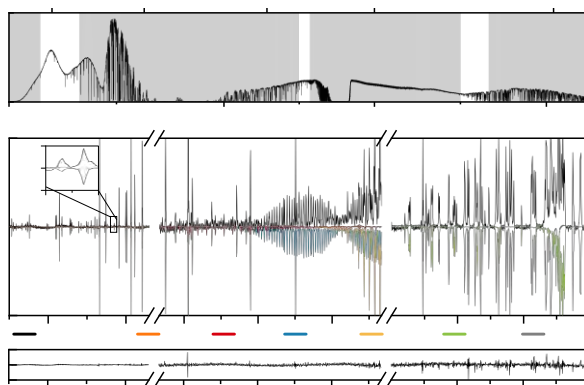
Most gases exhibit their strongest vibrational absorption in two regions of the mid-infrared (MIR) range: the functional group ( $3 - 4 \mu\text{m}$ ) and molecular fingerprint region ( $8 - 14 \mu\text{m}$ ). With broadband, high-resolution absorption spectroscopy on this spectral window, sensitive, multi-species gas sensing can be performed. However, until recently, coherent light sources with both the required broadband coverage, as well as the characteristics for sensitive measurements did not exist.

The emergence of a novel, ultra-broadband, MIR IDFG-based laser system enabled major advances in multi-species trace gas sensing. We demonstrated that the spectral coverage of  $2 - 11.5 \mu\text{m}$  of this source can be used for the simultaneous detection of many different gaseous compounds, ranging from hydrocarbons and oxides to small organic molecules [1]. The  $\sim 3 \text{ W}$  optical output, spatial coherence, and low noise of the source result in (sub)-ppb sensitivity for most of these compounds in measurement times varying from seconds to minutes.

Here, we will address two applications of spectroscopic measurements using this source. The first application is based on coherent open-path spectroscopy (COPS), in which the light beam is sent over an outdoor path to directly interact with the investigated gas medium. We demonstrated the performance of COPS in monitoring several emitted gases at a wastewater treatment plant (WWTP) [2]. Fig. 1 shows a typical COPS measurement, in which the high spectral resolution enables unambiguous identification and quantification of the different species over the broad spectral range of the source. Clear patterns in the emissions of  $\text{CO}_2$  and  $\text{CH}_4$  were found, while the observed concentrations of  $\text{N}_2\text{O}$ ,  $\text{CO}$ , and  $\text{NH}_3$  demonstrated no sustained emissions.

In the second application, we exploited the sensitive, multi-species detection capabilities of the system for exhaled breath analysis [3]. Human breath contains hundreds of compounds that can provide insights into metabolic processes in the body. The spectroscopic system was coupled to a dedicated breath-sampling system, designed to collect the alveolar portion of the exhalation. In several case studies, participants underwent an intervention, after which changes to the composition of their exhaled breath samples could be observed. These changes were resolved to specific molecular compounds and concentrations, providing direct evidence of the biochemical pathways and their relation to the intervention.

With the emergence of ultrabroadband MIR sources, opportunities arise for versatile systems that can be flexibly used for the (simultaneous) detection of many gaseous compounds.



**Fig. 1** Coherent open-path spectroscopy measurement (40-second average, 3 GHz spectral resolution) over a WWTP. a) Observed intensity spectrum. b) Absorbance spectrum with HITRAN spectra (in color, inverted). c) Residual of the fit.

## References

- [1] R. Krebbers, K. van Kempen, F. J. M. Harren, S. Vasilyev, I. F. Peterse, S. Lückner, A. Khodabakhsh, and S. M. Cristescu, "Ultra-broadband spectroscopy using a  $2-11.5 \mu\text{m}$  IDFG-based supercontinuum source," *Opt. Express* **32**(8), 14506–14520 (2024).
- [2] R. Krebbers, K. van Kempen, Y. Lin, J. Meurs, L. Hendriks, R. Aben, J. R. Paranaíba, C. Fritz, A. J. Veraart, A. Khodabakhsh, and S. M. Cristescu, "Ultra-broadband coherent open-path spectroscopy for multi-gas monitoring in wastewater treatment," *Environmental Science and Ecotechnology* **25**, 100554 (2025).
- [3] R. Krebbers, M. Huisman, K. van Kempen, J. Meurs, A. Khodabakhsh, S. M. Cristescu, "Broadband spectroscopic analyzer with an unprecedented profile of biomarkers in exhaled breath", *in preparation*.



# Multidimensional optical information detection

Fakun Wang<sup>1</sup>, Qi Jie Wang<sup>1,2\*</sup>

1. School of Electrical & Electronic Engineering, Nanyang Technological University, Singapore.

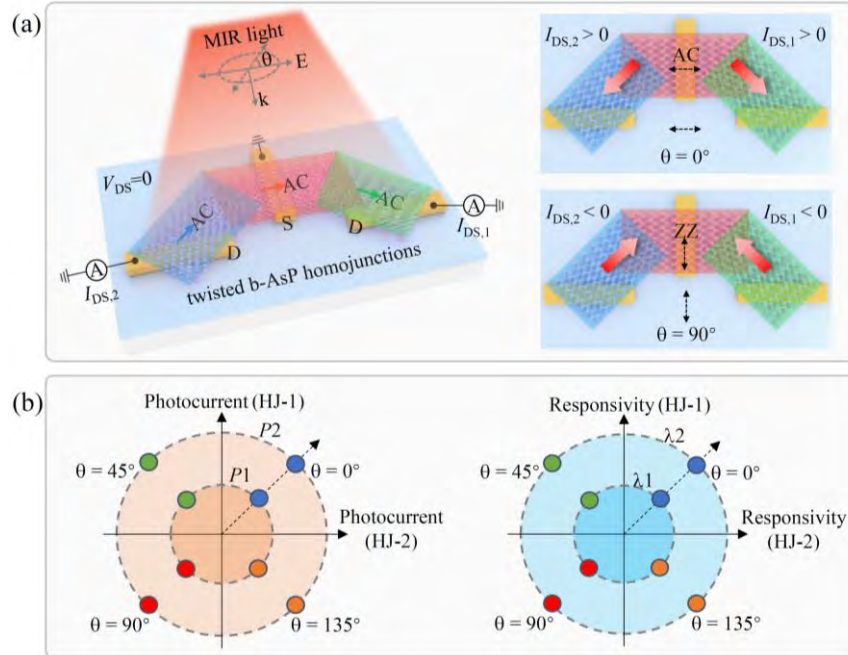
2. School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore.

Email: fakun.wang@ntu.edu.sg, qjwang@ntu.edu.sg

**Short abstract:** Multidimensional optical information, including intensity, polarization, and wavelength, can be simultaneously detected using double-twisted black arsenic-phosphorus (b-AsP) homojunctions, offering a versatile platform for advanced optical sensing applications.

Light field carrying multi-dimensional optical information (such as intensity, wavelength, and polarization) is essential for the important application scenarios such as environmental monitoring, thermal imaging, medical diagnosis, and free-space communications.<sup>1</sup> Simultaneous acquisition of these multi-dimensional optical information can provide many degrees of freedom for accurately identifying diverse targets and performing multifunctional tasks in parallel in complex environments.<sup>2</sup> However, this is difficult for most traditional optical detectors, because they can only detect information in one dimension, either wavelength, intensity or polarization due to the intercoupling of various polarization states with light intensity and wavelength.

Here, we demonstrate a multi-dimensional optical information detection device based on zero-bias double twisted b-AsP homojunctions,<sup>3</sup> where the photoresponse is dominated by the photothermoelectric effect. By employing bipolar and phase-offset polarization photoresponse, the device operated in the mid-infrared (MIR) range can simultaneously detect both the polarization angle and incident intensity information through direct measurement of the photocurrents of the double twisted b-AsP homojunctions. The device's responsivity allows for the retrieval of wavelength information, typically perceived as difficult to obtain. These demonstrations offer a promising approach for simultaneous detection of multi-dimensional optical information, indicating potential for diverse optical sensing applications.



**Fig. 1** (a) Schematic illustration of the designed multidimensional photodetectors consisting of double twisted b-AsP homojunctions. (b) Simultaneous detection of intensity (P), polarization ( $\theta$ ), and wavelength ( $\lambda$ ) by directly reading out the photocurrents and responsivities of the double twisted b-AsP homojunctions.

## References

- [1] F. K. Wang, F. C. Hu, et al. "A two-dimensional mid-infrared optoelectronic retina enabling simultaneous perception and encoding," *Nat. Commun.* **14**, 1938 (2023).
- [2] C. Ma, S. F. Yuan, P. Cheung, K. Watanabe, T. Tangiguchi, F. Zhang, and F. N. Xia, "Intelligent infrared sensing enabled by tunable moire quantum geometry," *Nature* **604**, 266-272 (2022).
- [3] F. K. Wang, S. Zhu, W. D. Chen, J. Y. Han, R. H. Duan, C. W. Wang, M. J. Dai, F. Y. Sun, Y. H. Jin, and Q. J. Wang, "Multidimensional detection enabled by twisted black arsenic-phosphorus homojunctions," *Nat. Nanotechnol.* **19**, 455-462 (2024).

# Raman spectroscopy for Clostridia produced hydrogen detection in milk

Daniele Barbiero<sup>1,2</sup>, Fabio Melison<sup>1</sup>, Lorenzo Cocola<sup>1</sup>, Massimo Fedel<sup>1</sup>, Christian Andrighetto<sup>3</sup>, Paola De Dea<sup>3</sup> and Luca Poletto<sup>1</sup>

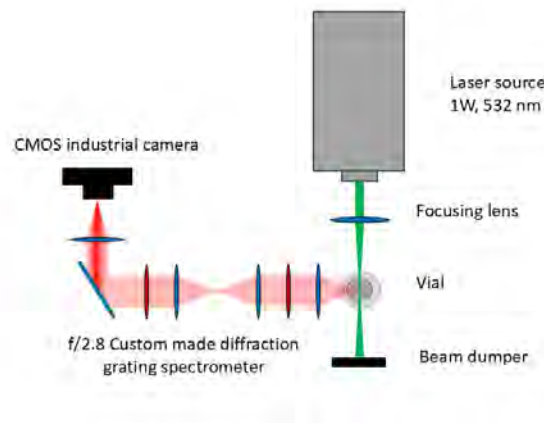
1. Institute for Photonics and Nanotechnologies, National Research Council, Via Trasea 7, 35131, Padua - Italy

2. University of Padova, Department of Information Engineering, Via Gradenigo 6/b, 35131, Padova, Italy

3. Veneto Agricoltura, Istituto per la Qualità e le Tecnologie Agroalimentari, Via San Gaetano 74, 36016 Thiene VI - Italy

**Short abstract:** Clostridia are bacteria that survive pasteurization and are known for producing hydrogen and carbon dioxide, causing late blowing defects in hard and semi-hard cheeses. Using a Raman spectroscopy-based instrument can reveal them selectively and well before traditional methods. This approach also allows to monitor the concentrations of hydrogen, nitrogen, oxygen, carbon dioxide simultaneously.

Clostridium are bacteria known to produce gases, especially carbon dioxide and hydrogen. However, the traditional method is not selective for these bacteria and is slow, while microbiological methods are too expensive to be used routinely. Raman spectroscopy is a valid solution because it allows the simultaneous measurement of different chemical species including carbon dioxide and hydrogen, the latter of which is impossible to measure using absorption spectroscopy in an optical path of the order of a centimeter. The setup consists of a laser source, whose beam is focused in the headspace of the vial under examination. Orthogonally, the scattered Raman light is collected by a custom made spectrometer coupled to a CMOS industrial camera. The setup is shown in figure 1.



**Fig. 1** Experimental setup.

The procedure is therefore similar to that applied in the classical most probable number (MPN) method but the positivity of a vial is determined on the basis of the hydrogen concentration present in the headspace of vials containing potentially infected milk. The system has been optimized to achieve a sensitivity of 29 spores per liter, which is of particular relevance given that nowadays there is no well-defined threshold to reject milk infected by clostridia but only an indicative value and would therefore be a valid tool to determine it. To limit the effect of fluorescence in the measurements, both hardware solutions, such as the use of two long-pass filters, and software solutions, such as the development of algorithms for the creation of spectra not saturated by fluorescence, were adopted. The instrument has been made portable and thermalized at 37 degrees. It allows to analyze 6 vials with a sampling every 5 minutes, or 24 vials with a sampling every half hour, proving effective given that the development dynamics takes from 48 to 72 hours of incubation.

## References

[1] Barbiero, D., Melison, F., Cocola, L., Fedel, M., Andrighetto, C., Dea, P. D., & Poletto, L. (2024). Raman Spectroscopy Applied to Early Detection of Clostridium Infection in Milk. In *Applied Spectroscopy* (Vol. 78, Issue 12, pp. 1256–1262). SAGE Publications. <https://doi.org/10.1177/00037028241252693>

# Topological ring resonator for refractive index sensing at telecommunication wavelength

Zaiyue Yang<sup>1</sup>, HongMing Fei<sup>1</sup>, Min Wu<sup>2</sup>, Han Lin<sup>3</sup>

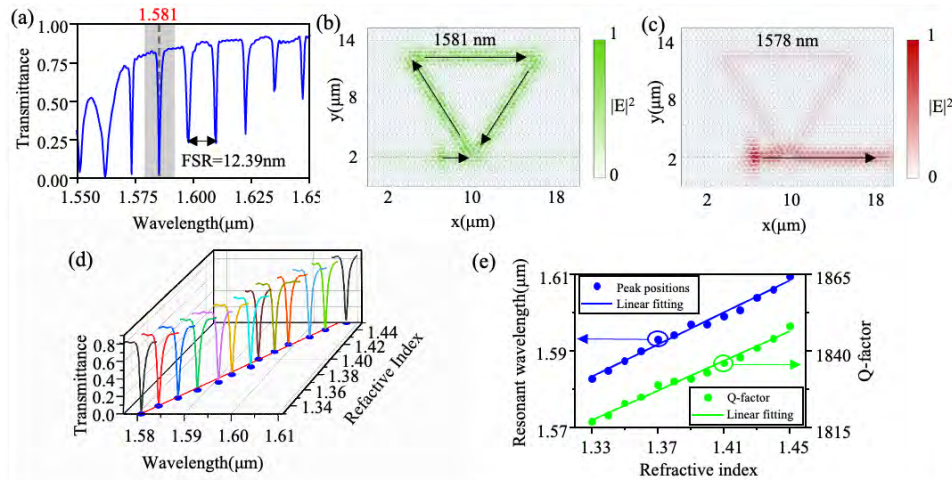
1. College of Physics and Optoelectronics, Taiyuan University of Technology, Taiyuan 030024, China

2. College of Information Engineering, Shanxi Vocational University of Engineering Science and Technology, Jinzhong 030619, China

3. Centre for Atomaterials and Nanomanufacturing, School of Science, RMIT University, Melbourne, Victoria 3000, Australia

**Short abstract:** We demonstrated topological refractive index sensors based on valley photonic crystal (VPC) ring resonator structures working at telecommunication wavelengths. These sensors have a phase shift of  $4.16\pi$  and a detection sensitivity of 208.09 nm/RIU (refractive index unit) with a detectable refractive index difference of 0.0044.

Ring resonators play an increasingly important role in biomedical sensing[1-3]. Conventional optical ring resonators based on waveguide structures have problems, such as large size and limited integrated density, and are easily influenced by external factors[4]. Therefore, new design principles are desired to achieve ultracompact biomedical sensors with high performance. This paper theoretically proposes a topological refractive index sensor based on the ring resonator at the telecommunication wavelength by detecting the shift of the resonance peaks in different refractive index environments to achieve refractive index sensing. Within the refractive index range of 1.33-1.45, it has a phase shift of  $4.16\pi$  and a sensitivity of up to 208.09 nm/RIU. It can detect a refractive index difference of 0.0044. Moreover, the combination of ring resonators of different sizes was explored, which can control the sensor's sensitivity through the FSR. In addition, the refractive index can also serve as an optical modulation mechanism to adjust the resonance peak. The structure proves the feasibility of designing biosensors based on topological ring resonators. At the same time, this structure can be manufactured using the existing mature CMOS nanofabrication process, so it is suitable for experimental demonstration.



**Fig. 1** (a) Transmission spectrum of a ring resonator with solution refractive index of 1.33. (b) and (c) are the electric field intensity distributions of the ring resonator at 1578 nm and 1581 nm with the solution refractive index of 1.33. (d) Transmission spectra of the resonance peak of the ring resonator at 1581 nm with the solution refractive index of 1.33 in different refractive index solutions. (e) Relationship between the resonance wavelength (1581 nm with the refractive index of 1.33) and linear fitting.

## References

- [1] Song, S.; Xu, H.; Fan, C. H., "Potential diagnostic applications of biosensors: current and future directions". *Int. J. Nanomed.*, **1** (4), 433-440(2006).
- [2] Pourbasheer, E.; Azari, Z.; Ganjali, M. R., "Recent Advances in Biosensors Based Nanostructure for Pharmaceutical Analysis". *Curr. Anal. Chem.*, **15** (2), 152-158(2019).
- [3] Ali, L.; Mohammed, M. U.; Khan, M.; Yousuf, A. H. B.; Chowdhury, M. H., "High-Quality Optical Ring Resonator-Based Biosensor for Cancer Detection". *IEEE Sensors Journal*, **20** (4), 1867-1875(2020).
- [4] Z. L. Rani, X. He, Y. J. Rao, D. Sun, X. J. Qin, D. B. Zeng, W. W. Chu, X. K. Li, and Y. B. Wei, "Fiber-Optic Microstructure Sensors: A Review", *Photonic Sensors* **11**, 227-261 (2021).

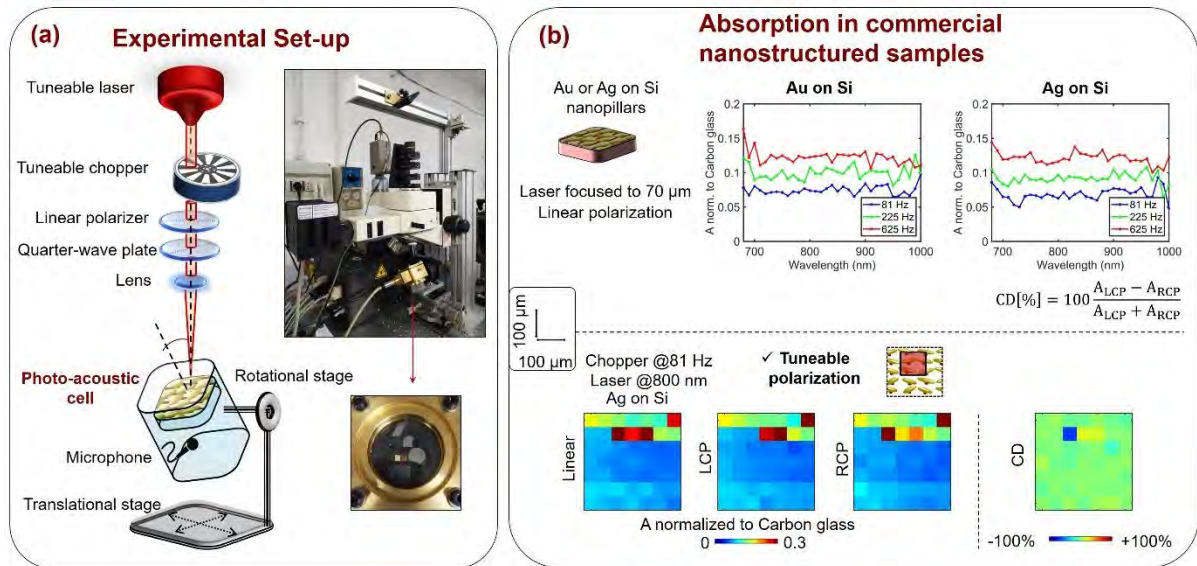
# Photo-acoustics meets nanoplasmonics: widely tuneable photo-acoustic spectroscopy on commercial nanostructured samples

Emilija Petronijevic<sup>1</sup>, Claudia Skubisz<sup>1</sup>, Grigore Leahu<sup>1</sup>, Roberto Li Voti<sup>1</sup>, Concita Sibilica<sup>1</sup>, Alessandro Belardini<sup>1</sup>

*1. SBAI Department, Sapienza Università di Roma, Via Antonio Scarpa 14-16, 00161 Rome – Italy*

**Short abstract:** Photo-acoustic spectroscopy (PAS) is a low-cost, scattering-free and non-destructive method of measuring nanomaterial absorption. We enrich PAS with many degrees of freedom: laser wavelength, polarization, direction, focus, possibilities of spatial and frequency mapping, and a microscope. We show its potential in characterizing both commercial nanostructures.

We have previously used photo-acoustic technique as means of characterizing absorption and chirality of various specially designed nanostructures [1] and metamaterials [2] at single wavelengths. However, for more general investigation of resonant absorption in nanostructured media, a widely tuneable laser excitation is needed [3]. In this study, we enrich the PAS set-up with a widely tuneable laser, covering the near-infrared (680-1080 nm) and visible (340-540 nm) ranges. Moreover, our set-up has tuneable chopper frequency, light polarization and direction, beam waist control, and the possibility to spatially map the surfaces. General schematic of the set-up is shown in the left part of Fig. 1(a), while the right part shows images of the added microscope (top), and the photo-acoustic cell with many samples (bottom). Fig. 1(b) shows spectral and spatial absorption mapping in commercial achiral nanostructured samples: Au- or Ag-covered Si nanopillars [4]. The absorption spectra for three chopper frequencies are normalized to the absorption spectra of a Carbon glass sample obtained at the same frequency; we note that the increase of frequency increases the normalized absorption, top of Fig. 1(b). In the bottom of Fig. 1(b), we perform spatial mapping of absorption for a light beam at 800 nm, focused to 70  $\mu\text{m}$ , at chopper frequency of 81 Hz, for three polarizations; the mapping step in both planar directions is 100  $\mu\text{m}$ . This shows potential to map both uniformity of the sample, and the differential absorption of opposite circular polarizations, i.e. circular dichroism (CD).



**Fig. 1** (a) Photo-acoustic set-up (left) and images of the additional microscope (right top) and photo-acoustic cell with various samples (right bottom). (b) Wavelength and spatial mapping of commercial nanostructured samples: Au- or Ag-covered Si nanopillars. Top: absorption spectra for three chopper frequencies. Bottom: spatial mapping at the wavelength of 800 nm and chopper frequency of 81 Hz, for three polarizations, and the corresponding CD. All the absorption data are normalized to the absorption of a Carbon glass sample at the same chopper frequency.

We strongly believe that this enriched PAS set-up can be used to sensitively map absorption and chirality of nanostructured media in a broad wavelength range and with many degrees of freedom.

## References

- [1] G. Leahu et al, "Evidence of Optical Circular Dichroism in GaAs-Based Nanowires Partially Covered with Gold", *Adv. Opt. Mater.* 5(16), 1601063 (2017).
- [2] E. Petronijevic et al, "Photo-acoustic detection of chirality in metal-polystyrene metasurfaces", *Appl. Phys. Lett.* 114, 053101 (2019).
- [3] E. Petronijevic et al, "Extrinsic chirality tailors Stokes parameters in simple asymmetric metasurfaces", *Nanoscale* 16, 16477 – 16484 (2024).
- [4] R. R. Jones et al, "Chirality conferral enables the observation of hyper-Raman optical activity", *Nat. Photon.* 18(9), 982–989 (2024).



# Wavelength Modulation Spectroscopy for the study of nitrogen oxide concentration after electric discharges simulating lightning

Claire Birot<sup>1</sup>, François Mayer<sup>1</sup>, Gautier Vilmart<sup>1</sup>, Clément Zaepffel<sup>1</sup>, Myriam Raybaut<sup>1</sup>,  
Frédéric Champagnat<sup>2</sup>, Magalie Buguet<sup>1</sup>, Christophe Brossard<sup>1</sup>, Aurélien Plyer<sup>2</sup>

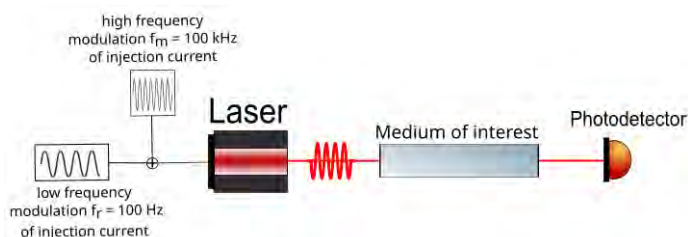
1. DPHY, ONERA, Université Paris-Saclay, 91120, Palaiseau, France

2. DTIS, ONERA, Université Paris-Saclay, 91120, Palaiseau, France

**Short abstract:** Wavelength Modulation Spectroscopy is studied in the case of Nitrogen Oxide production after an electric discharge, for atmospheric studies linked to NO production due to lightning.

Optical diagnostic techniques such as TDLAS are commonly used to probe media of interest in a non-intrusive way. This method, based on the Beer Lambert law, consists in propagating through the investigated medium a laser beam emitted by a diode laser tunable in wavelength. The measured absorption spectrum depends on the spatial distribution of temperature, concentration and pressure. The processing of this spectrum allows to determine integrated values of temperature and concentration of the probed species. Main advantages of TDLAS are that the concentration deduced is absolute, its relative ease of implementation and the high repetition rate possible (10 kHz or more). However, TDLAS is sensitive to vibrations and parasitic etalon effects created by parallel surfaces, which can lead to signal distortion and decrease the measurement accuracy.

WMS (Wavelength Modulation Spectroscopy) aims to reduce sensitivity to such distortions [1]. As illustrated in Figure 1, this technique involves modulating the diode's injection current with a high-frequency sinusoidal signal. Heterodyne detection allows to reject low frequency noise (i.e. lower than the high modulation frequency), and a normalization step allows to take into account the spectrum distortion. In this study, high frequency modulation is implemented with a Quantum Cascade Laser to target the nitric oxide (NO) molecule.



**Figure 1 :** Principle of Wavelength Modulation Spectroscopy



**Figure 2 :** Experimental setup of nitrogen oxide concentration measurement

NO is of particular interest because it contributes to the formation of tropospheric ozone, a greenhouse gas naturally produced after electrical discharges such as lightning. We applied the high frequency modulation technique to measure NO concentrations generated by an electric discharge in the ONERA GRIFON test facility (shown in Figure 2). The GRIFON facility allows to the production of discharges at different pressures, representatives of different atmospheric conditions. We thus performed tests at three different pressures (from 0.2 bar to 1 bar), with four values of currents intensities (from 13 kA to 90 kA). This study aims to help enhance NO quantification by capturing its temporal dynamics, and by providing new measurements to reduce the uncertainties surrounding NO concentrations created by lightning [2].

## References

- [1] D. S. Bomse, A. C. Stanton, et J. A. Silver, « Frequency modulation and wavelength modulation spectroscopies: comparison of experimental methods using a lead-salt diode laser », *Appl. Opt.*, vol. 31, févr. 1992, doi: 10.1364/AO.31.000718.
- [2] S. Verma, P. K. Yadava, D. M. Lal, R. K. Mall, H. Kumar, et S. Payra, « Role of Lightning NOx in Ozone Formation: A Review », *Pure Appl. Geophys.*, vol. 178, avr. 2021, doi: 10.1007/s00024-021-02710-5.

# Advanced Spectroscopic Techniques



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# Semiconductor quantum walk combs for spectroscopy and telecommunication applications

J. Faist, I. Heckelmann, A. Dikopoltsev, B. Marzban, L. Miller, M. Montesinos-Ballister, M. Bertrand, . Cargioli, D. Piciocchi, V. Degiorgio, M. Beck, G. Scalari

*IQE, ETH Zürich, Switzerland*

*Author e-mail address: Jerome.faist@phys.ethz.ch*

The random walk is a fundamental concept in mathematics and physics that describes a walker taking random steps in a discretized space. While the spread of a classical random walker is characterized by a square root standard deviation after  $N$  steps it is surpassed by its quantum counterpart, in which the standard deviation of the position scales linearly with the number of steps. We recently showed that the concept of quantum walk[1] can be applied to the synthetic dimension formed by the modes of a resonator where a phase modulation induced, for instance, through the electro-optical effect or the laser's pump can introduce coupling in the chain, giving rise to continuous-time quantum walk dynamics. Qualitatively, dispersion induces an effective potential well in frequency space whereas the width of the band created by modulation limits the maximum achievable the system's bandwidth equal to  $2c/\pi n \sqrt{(M/\beta)}$  where  $M$  the modulation depth and  $\beta$  the GVD parameter.

This system can be analogously mapped to a quantum harmonic oscillator[2]. We demonstrate both theoretically and experimentally that the full potential of the synthetic frequency lattice can be unlocked by employing ultrafast saturable gain. The giant nonlinearity of such gain locks the resonator modes and effectively counteracts the dispersion. This is in great contrast with the situation of slow gain where, as was shown many years ago, only the fundamental mode is the Gaussian-shaped fundamental mode of the parabolic potential[2].

Laser based on semiconductors active regions are, in general, excellent candidates to realize quantum walk combs, as they exhibit very naturally both the phase modulation as well as the fast gain saturation which are both key for the operation of the device. It is also true in interband devices despite the relatively long spontaneous emission time[3]. The coupling between the real and imaginary part of the gain, responsible for the linewidth enhancement factor, will ensure that a modulation of the gain will also generate the phase modulation necessary for the proliferation of the modes.

We report the operation of such combs across the electromagnetic spectrum from the Terahertz to the near-infrared, demonstrating the universal character of the quantum walk comb in semiconductor lasers. Quantum walk combs are equally relevant for applications in sensing or telecommunication as well as a platform for emulation of quench dynamics, taking advantage of the liquid-like properties of light in a fast gain medium[4].

The quantum walk comb controllability is especially valuable for applications in telecommunications and spectroscopy.

## Bibliography

- [1] I. Heckelmann, M. Bertrand, A. Dikopoltsev, M. Beck, G. Scalari, and J. Faist, "Quantum walk comb in a fast gain laser," *Science*, vol. 382, no. 6669, pp. 434–438, Oct. 2023, doi: [10.1126/science.adj3858](https://doi.org/10.1126/science.adj3858).
- [2] H. Haus, "A theory of forced mode locking," *IEEE Journal of Quantum Electronics*, vol. 11, no. 7, pp. 323–330, Jul. 1975, doi: [10.1109/JQE.1975.1068636](https://doi.org/10.1109/JQE.1975.1068636).
- [3] B. Marzban, L. Miller, A. Dikopoltsev, M. Bertrand, G. Scalari, and J. Faist, "A Quantum Walk Comb Source at Telecommunication Wavelengths," Nov. 13, 2024, *arXiv*: arXiv:2411.08280. doi: [10.48550/arXiv.2411.08280](https://doi.org/10.48550/arXiv.2411.08280).
- [4] A. Dikopoltsev *et al.*, "Quench dynamics of Wannier-Stark states in an active synthetic photonic lattice," May 08, 2024, *arXiv*: arXiv:2405.04774. doi: [10.48550/arXiv.2405.04774](https://doi.org/10.48550/arXiv.2405.04774).

# Comb-linked cavity ring-down spectroscopy: probing ultra-weak absorption from the deep-ultraviolet to the mid-infrared

Livio Gianfrani

*Dipartimento di Matematica e Fisica, Università degli Studi della Campania Luigi Vanvitelli, Viale Lincoln 5 - 81100, Caserta – Italy*

**Short abstract:** I will report on current experiments of ultrasensitive detection of atomic and molecular absorption by means of cavity ring-down spectroscopy assisted by the technology of optical frequency combs. A broad spectrum of applications will be covered: from trace water detection in high purity gases to partial pressure measurements of residue hydrocarbons in ultra-high vacuum environments.

Cavity ring-down spectroscopy (CRDS) is a highly sensitive laser-based technique for probing the atomic and molecular constituents of any gaseous medium that is confined inside a high-finesse optical cavity. It consists in measuring the rate of decay of light intensity on the transmission from a stable optical resonator, once the incident laser radiation is instantaneously switched off. The recent combination of CRDS with frequency comb technologies has further enhanced its capabilities, adding metrology-grade qualities to spectroscopic determinations, such as transition frequencies and line intensity factors [1]. High detection sensitivity in conjunction to high precision and accuracy enables for fundamental tests and measurements in a few selected molecules of fundamental importance for understanding quantum chemistry theories or testing quantum electrodynamics [2-4]. On the other hand, CRDS is currently experiencing new frontiers of applications. A first example is given by residual water concentration measurements in ultra-high-purity gases that are needed in manufacturing processes of the semiconductor industry to meet the quality requirements [5, 6]. Another example concerns the first application of CRDS to ultra-high vacuum environments that are expected in the next generations of ground-based interferometric gravitational-wave detectors, such as the Einstein Telescope. In this regard, it is important to measure the partial pressure of the volatile residue of hydrocarbons at the level of  $10^{-12}$  mbar and even below.

I will report on recent results in this research field, as obtained at the CIRCE laboratories of the Università degli Studi della Campania, in Caserta. Successful experiments make use of a variety of lasers, including external-cavity diode lasers, interband cascade lasers, as well as coherent sources based on nonlinear mixing schemes, thus covering a wide interval of wavelengths, from the deep-ultraviolet to the mid-infrared. Target molecules include hydrogen, water, acetylene, nitrous oxide and carbon dioxide.

## References

- [1] L. Gianfrani, S.-M. Hu, W. Ubachs, “Advances in cavity-enhanced methods for high precision molecular spectroscopy and test of fundamental physics”, *La Rivista del Nuovo Cimento* **47**, 229–298 (2024).
- [2] E. Fasci, A. Castrillo, H. Dinesan, S. Gravina, L. Moretti, L. Gianfrani, “Precision spectroscopy of HD at  $1.38\ \mu\text{m}$ ”, *Phys. Rev. A* **98**, 22516 (2018).
- [3] A. Castrillo, E. Fasci, T. Furtenbacher, V. D’Agostino, M.A. Khan, S. Gravina, L. Gianfrani and A.G. Császár, “On the  $^{12}\text{C}_2\text{H}_2$  near-infrared spectrum: absolute transition frequencies and an improved spectroscopic network at the kHz accuracy level”, *Phys. Chem. Chem. Phys.* **25**, 23614–23625 (2023).
- [4] Qian-Hao Liu, Yan Tan, Cun-Feng Cheng, and Shui-Ming Hu, “Precision spectroscopy of molecular hydrogen”, *Phys. Chem. Chem. Phys.* **25**, 27914 (2023).
- [5] E. Fasci, M. A. Khan, V. D’Agostino, S. Gravina, V. Femicola, L. Gianfrani, and A. Castrillo, “Water vapor concentration measurements in high purity gases by means of comb assisted cavity ring down spectroscopy”, *Sens. Actuators A - Phys.* **362**, 114632 (2023).
- [6] A. Castrillo, M.A. Khan, E. Fasci, V. D’Agostino, S. Gravina, and L. Gianfrani, *Optica* **11**, 1277-1284 (2024).



# Intracavity cantilever-based photoacoustic sensors: exploring unconventional regimes bringing together sensitivity and resolution

Jacopo Pelini<sup>a</sup>, Stefano Dello Russo<sup>b</sup>, Zhen Wang<sup>c</sup>, Iacopo Galli<sup>a</sup>, Pablo Cancio Pastor<sup>a</sup>, Marica Canino<sup>d</sup>, Alberto Roncaglia<sup>d</sup>, Wei Ren<sup>c</sup>, Paolo De Natale<sup>a</sup>, Mario Siciliani de Cumis<sup>a,b</sup>, and Simone Borri<sup>a,\*</sup>

<sup>a</sup> CNR-INO - Istituto Nazionale di Ottica, and LENS, Via Carrara 1, 50019 Sesto Fiorentino FI, Italy

<sup>b</sup> ASI Agenzia Spaziale Italiana - Centro di Geodesia Spaziale, Località Terlecchia, 75100 Matera, Italy

<sup>c</sup> The Chinese University of Hong Kong, New Territories, Hong Kong SAR, China

<sup>d</sup> CNR-IMM - Istituto per la Microelettronica e Microsistemi, Via P. Gobetti 101, 40129 Bologna, Italy

\* [simone.borri@ino.cnr.it](mailto:simone.borri@ino.cnr.it)

**Short abstract:** Through the combination with mid infrared sources and high finesse cavities, photoacoustic sensors have achieved unprecedented sensitivity levels. The availability of a high intracavity optical power opens unexplored perspectives for photoacoustic sensors, allowing to exploit unconventional regimes bringing together sensitivity and resolution. Our latest results are here presented and discussed.

Among trace-gas optical sensing techniques, photoacoustic sensors stand for their unique combination of sensitivity and flexibility. Thanks to the high number of degrees of freedom offered by this technique, ultra-high detection sensitivities at the part-per-trillion (ppt) levels or below [1-3] have been demonstrated by optimizing individually and simultaneously all the key components of the sensing system, such as exploiting mid-infrared semiconductor lasers as the excitation sources and enhancing the available interacting radiant power via high-finesse optical cavities.

Here we present our latest results on advanced configurations of a cantilever-based sensor, combining the advantages of the photoacoustic technique with the sensitivity enhancement provided by a doubly-resonant (acoustic and optical) system. In our setup, a 4.5- $\mu\text{m}$  CW quantum cascade laser is used to address fundamental rovibrational transitions of N<sub>2</sub>O, selected as target molecule to test the sensor performance. Several silicon MEMS cantilevers have been tested as acoustic transducers, including standard rectangular cantilevers and structures characterized by unconventional shapes. The cantilever displacement is measured with a custom-designed balanced Michelson interferometer. The different cantilever performances have been compared [4] and the most promising structure has been used to study the ultimate detection sensitivity of the sensor. In addition, the signal enhancement provided by the use of dual-tube acoustic resonators has also been investigated [5].

Particularly interesting scenarios open up when these systems are combined with high-finesse optical cavities. Here, the photoacoustic signal enhancement due to high intracavity optical powers can be explored. Moreover, the generally higher photoacoustic signal guaranteed by this advanced configuration allows to explore unconventional regimes as low sample pressures, which in standard photoacoustic sensors are out of range due to the suppressed acoustic wave generation and transmission.

In the standard “high-pressure” regime, optimal for in-field environmental monitoring and air-quality analysis, our setup achieves detection sensitivities down to tens of ppt [6]. Thanks to the cavity power build-up factor and the strong mid IR molecular transitions, the sensor can be operated also at extremely low power levels (tens of  $\mu\text{W}$ ) still maintaining detection sensitivity at the ppb level. Finally, low sample pressure regimes can be explored, allowing to record sub-Doppler absorption profiles and opening exciting new perspectives for photoacoustic sensors towards the combination of high sensitivity and high resolution molecular sensing.

## References

- [1] S. Borri, P. Patimisco, I. Galli, D. Mazzotti, G. Giusfredi, N. Akikusa, M. Yamanishi, G. Scamarcio, P. De Natale, and V. Spagnolo, *Appl. Phys. Lett.* 104, 091114 (2014).
- [2] T. Tomberg, T. Hieta, M. Vainio, and L. Halonen, *Analyst* 144, 2291 (2019).
- [3] Z. Wang, Q. Wang, H. Zhang, S. Borri, I. Galli, A. Sampaolo, P. Patimisco, V.L. Spagnolo, P. De Natale, and W. Ren, *Photoacoustics* 27, 100387 (2022).
- [4] J. Pelini, S. Dello Russo, I. Lopez Garcia, M. Canino, A. Roncaglia, P. Cancio Pastor, I. Galli, W. Ren, P. De Natale, S. Borri, and M. Siciliani de Cumis, *Photoacoustics* 38, 100619 (2024).
- [5] S. Dello Russo, J. Pelini, I. Lopez Garcia, M. Canino, A. Roncaglia, P. Cancio Pastor, I. Galli, P. De Natale, S. Borri, and M. Siciliani de Cumis, *Photoacoustics* 40, 100644 (2024).
- [6] J. Pelini, S. Dello Russo, Z. Wang, I. Galli, P. Cancio Pastor, I. Lopez Garcia, M. Concetta Canino, A. Roncaglia, N. Akikusa, W. Ren, P. De Natale, M. Siciliani de Cumis, and S. Borri, *Sens. Actuators B Chem.* 430, 137313 (2025).

# Quantum walk comb FM spectroscopy

Davide Pinto<sup>1</sup>, Ina Heckelmann<sup>1</sup>, Mathieu Bertrand<sup>1</sup>, Uwe Schmitt<sup>2</sup>, Mattias Beck<sup>1</sup>, Giacomo Scalari<sup>1</sup>, Jérôme Faist<sup>1</sup>

1. Institute for Quantum Electronics, ETH Zürich, Auguste-Piccard-Hof 1, 8093 Zürich, Switzerland

2. Scientific IT Services, ETH Zürich, Binzmühlestrasse 130, 8092 Zürich, Switzerland

**Short abstract:** We present a novel all-electronic spectroscopic method based on a quantum walk QCL comb for solvents detection in the fingerprint region. Spectral shaping of the comb source was achieved by frequency modulation of the RF-injected signal, allowing for fast and broadband detection of the analyte's absorption features.

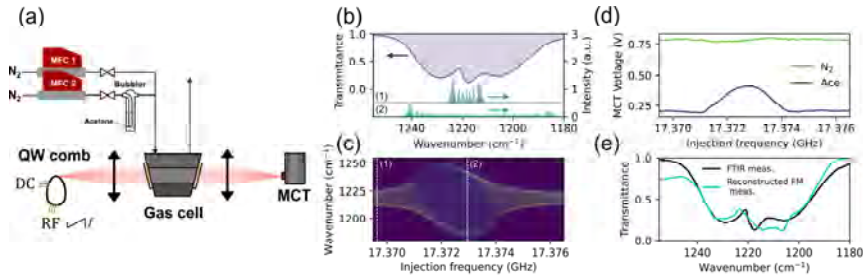
Quantum walk comb lasers are a promising coherent broadband source of radiation [1], which feature a stable, predictable, and tunable spectrum. The quantum walk is induced by coupling the frequency ladder modes of an active optical ring cavity via RF-injection. The active platform is a Quantum Cascade Laser (QCL), a device that relies on intersubband transitions with an extremely fast recovery time ( $\sim$  ps scale). For generating this new type of frequency combs, the fast gain recovery time is essential to stabilize it towards the state of highest bandwidth. For their unique properties, frequency combs have been extensively applied to spectroscopy. Comb-based spectrometers retrieve the information stored in each comb line after interacting with the sample. However, this usually implies the use of bulky optical components, such as gratings or moving parts - as in Fourier Transform spectroscopy - or the need for a matched pair of combs for dual-comb spectroscopy [2,3].

In this work, we present a novel spectroscopic approach that requires a single quantum walk comb for fast and broadband sensing, in a highly simplified experimental setup. Our technique relies on the tunability of the comb spectrum induced by FM modulation of the RF frequency ( $f$ ), swept (at kHz up to MHz rates) across the resonance frequency, while the integrated optical power is collected on a photodetector ( $\mathbf{b}(f)$ ). With the knowledge of the spectrum tuning properties, the transmittance ( $\mathbf{x}(v)$ ) of the sample can be retrieved by inverting the matrix that describes the tuning properties of the laser  $\mathbf{M}(v, f)$ :

$$\mathbf{x}(v) = \mathbf{M}^{-1}(v, f) \mathbf{b}(f) \quad (1)$$

We give the first demonstration of an FM quantum walk comb spectrometer for the detection of gaseous acetone in the fingerprint region. The experimental setup (Fig.1(a)) features a ring QCL emitting around 1220  $\text{cm}^{-1}$ , with a spectral coverage of  $\sim 70 \text{ cm}^{-1}$  and a spectral spacing of  $0.6 \text{ cm}^{-1}$ . A mixture of gaseous acetone and  $\text{N}_2$  was flushed in a 5 cm long gas cell. The collimated QCL beam was focused onto an MCT after passing through the gas cell and the MCT voltage was recorded for data processing.

The QW comb emission was tuned at kHz rate by acting on the RF injection frequency as shown in Fig.1(c), allowing for fast averaging of the spectroscopic measurement. Preliminary measurements for the nitrogen and the acetone-filled gas cell are shown in Fig.1(d). The peculiar shape of the sample spectrum comes from an interplay between the absorption feature and the varying intensity distribution of the comb spectrum (as displayed in Fig.1(b)). The absorption feature was reconstructed (Fig.1(e)) by multiplying the regularized inverted calibration matrix ( $\mathbf{M}^{-1}(v, f)$ ) with the FM-measurement ( $\mathbf{b}(f)$ ).



**Fig. 1** (a) Schematic of the experimental setup used for single QW comb spectroscopy. (b) Two representative spectra compared with the investigated acetone absorption feature. (c) Spectral shaping of the QW laser as a function of the RF injection frequency. (d) Spectroscopic measurement of pure nitrogen and a mixture containing of acetone in nitrogen. (e) FTIR and reconstruction measurements of the acetone feature.

## References

- [1] I. Heckelmann, M. Bertrand, A. Dikopoltsev, M. Beck, G. Scalari, and J. Faist, 'Quantum walk comb in a fast gain laser', Science, vol. 382, no. 6669, pp. 434–438, Oct. 2023.
- [2] Mandon, J., Guelachvili, G. and Picqué, N., 'Fourier transform spectroscopy with a laser frequency comb'. Nature Photonics 3, 99–102 (2009).
- [3] N. Picqué, T.W. Hänsch, Frequency comb spectroscopy, Nature Photonics 13, 146–157 (2019).

# Development of a novel GC-QEPAS sensing system for Volatile Organic Compounds detection

Lavinia Anna Mongelli<sup>1</sup>, Arianna Elefante<sup>2</sup>, Giansergio Menduni<sup>1</sup>, Marilena Giglio<sup>1</sup>, Vincenzo Spagnolo<sup>1</sup> and Angelo Sampaolo<sup>1</sup>.

1. PolySense Lab-Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari, Italy

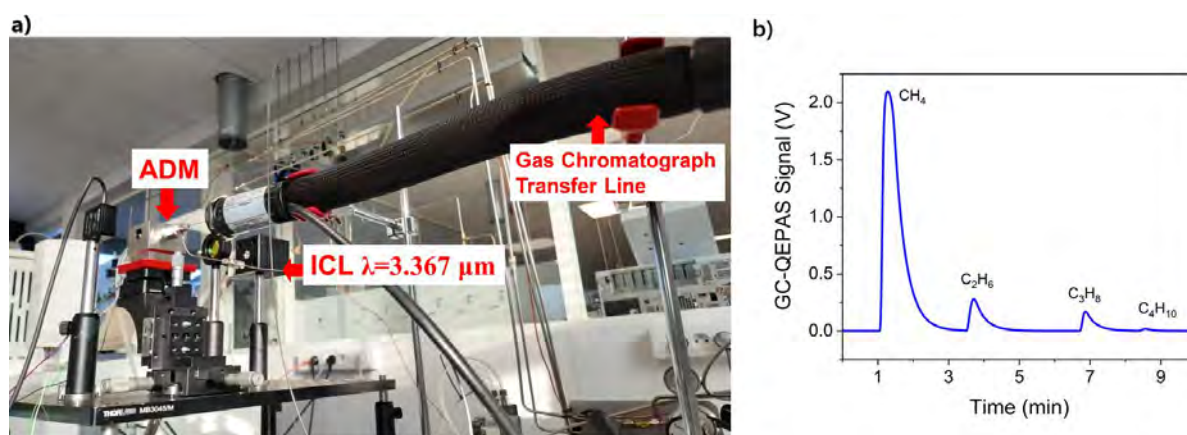
2. Institute for Photonics and Nanotechnologies (IFN), National Research Council, Via Amendola 173, Bari, Italy

**Short abstract:** This work presents an innovative analytical system combining gas chromatography (GC) with Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) sensor for volatile organic compounds detection. An interband cascade laser (ICL) emitting at 3.367  $\mu\text{m}$  was employed, with light alkanes - methane, ethane, propane, and butane - selected as case studies to evaluate the detection performance.

Volatile organic compounds (VOCs) are chemicals that can evaporate at atmospheric conditions of temperature and pressure acting as markers of both air pollution and quality, process contamination and authenticity in food production.

Among optical sensors, Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) has emerged as a powerful method for trace gas detection. In photoacoustic spectroscopy, gas molecules absorb modulated laser light, which is converted to heat. The modulated absorption generates pressure waves, detected by a quartz tuning fork and transduced into an electric signal, thanks to the piezoelectric effect. QEPAS sensors can identify different VOCs targeting specific spectral features, enabling sensitive, rapid, and non-destructive measurements. However, optical spectroscopy for VOCs often faces interference from atmospheric compounds (e.g.,  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CH}_4$ ), and overlapping absorption features, common among similar molecules, such as ethane, propane, and butane [1]. This study focuses on the selective detection of light alkanes—methane, ethane, propane and butane—using an innovative detection system that combines gas chromatography (GC) with QEPAS sensor.

The core innovation lies in integrating the GC technique, which provides temporal separation of eluted molecules, with the QEPAS infrared analysis technique, enabling highly sensitive measurements of absorber concentrations. The laser source employed for this investigation consisted in an interband cascade laser (ICL) emitting at a central wavelength of  $\lambda=3.367\ \mu\text{m}$  and capable to target an intense mid-infrared absorption band of propane [2]. A photo of the developed experimental setup core is shown in Fig. 1a.



**Fig. 1** (a) Photograph of the experimental setup core. ADM, Acoustic Detection Module; ICL, Interband Cascade Laser. (b) GC-QEPAS spectra of a sample comprising 90% methane, 5% ethane, 0.2% propane, and butane at a concentration below 0.001. The measurements were performed at ambient condition of temperature and pressure.

After identifying the optimal operating conditions, the GC-QEPAS signal was acquired by locking the laser current at 80 mA to align with the propane absorption peak. The chromatogram in Fig. 1b illustrates the individual detection and quantitative analysis of compounds eluted over time by gas chromatography. The trace corresponds to a sample containing 90% methane, 5% ethane, 0.2% propane, and less than 0.001% butane. The SNR measured for this last molecules is 60, demonstrating the high sensitivity and the capability of the sensor to accurately detect components even in the presence of complex chemical interferences.

## References

- [1] A. F. P. Cantatore *et al.*, "Methane, Ethane, and Propane Detection Using a Quartz-Enhanced Photoacoustic Sensor for Natural Gas Composition Analysis," *Energy and Fuels*, Jan. 2024, doi: 10.1021/acs.energyfuels.4c03726.
- [2] K. Kinjalk *et al.*, "Highly selective and sensitive detection of volatile organic compounds using long wavelength InAs-based quantum cascade lasers through quartz-enhanced photoacoustic spectroscopy," *Appl Phys Rev*, vol. 11, no. 2, Jun. 2024.

# Photothermal and Photoacoustic Spectroscopy



Biorobotics Research &  
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Digital Driven Diagnostics,  
prognostics and therapeutics  
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Ministry of Foreign Affairs  
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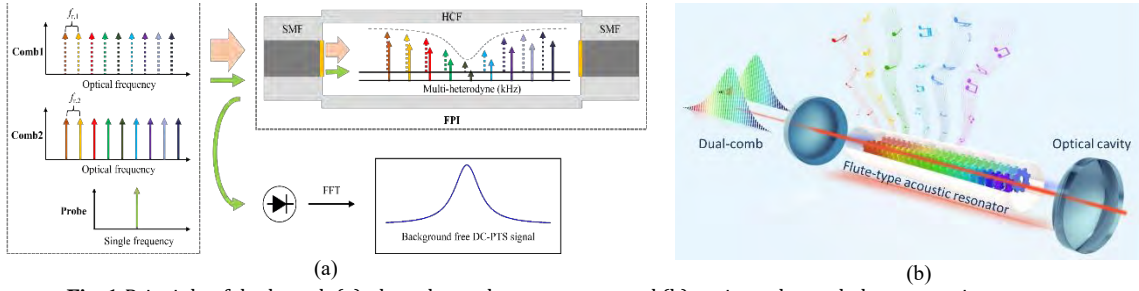
# Dual-Comb Photothermal and Photoacoustic Spectroscopy

Wei Ren

Department of Mechanical and Automation Engineering, The Chinese University of Hong Kong, New Territories, Hong Kong SAR, China

**Short abstract:** Dual-comb spectroscopy (DCS) has become a powerful tool in various fields to provide high-precision and broadband spectroscopic measurements. I will discuss our recent innovations in dual-comb photothermal and photoacoustic spectroscopy, enabling highly powerful analytical tools for broadband, high-sensitivity, and background-free spectroscopic measurements.

Laser spectroscopic techniques using optical frequency combs (OFCs) with many equally spaced, mutually coherent, narrow spectral lines are attracting a lot of attention. Dual-comb spectroscopy (DCS) by adopting two OFCs with slightly different repetition rates is an emerging tool that performs Fourier transform spectroscopy without any moving parts. Traditional DCS is conducted by measuring the transmitted comb light intensity using a fast photodetector, in which the absorption information has to be extracted from the irregular background signal, leading to the limitation of the detection sensitivity. In this talk, I will discuss our recent innovations in dual-comb photothermal and photoacoustic spectroscopy [1,2], enabling highly powerful analytical tools for broadband, high-precision and high-sensitivity spectroscopic measurements. This advancement in spectroscopy paves the way for a wider range of gas sensing applications in energy, environment and safety management.



**Fig. 1** Principle of dual-comb (a) photothermal spectroscopy and (b) cavity-enhanced photoacoustic spectroscopy.

## References

- [1] Q. Wang, Z. Wang, H. Zhang, S. Jiang, Y. Wang, W. Jin, and W. Ren, "Dual-comb photothermal spectroscopy," *Nat. Commun.* **13**, 2181 (2022).
- [2] Z. Wang, Q. Nie, H. Sun, Q. Wang, S. Borri, P. D. Natale, and W. Ren, "Cavity-enhanced photoacoustic dual-comb spectroscopy," *Light: Sci. Appl.* **13**, 11 (2024).

# NDT by Photoacoustic and Photothermal Techniques: Recent Advances and Perspectives

R. Li Voti, G. Leahu, E. Petronijevic, C. Skubisz, A. Maurizi, G.alle, G. Cesarini,  
M.C. Larciprete, M. Centini, A. Belardini, C. Sibilial

*Sapienza Università di Roma, Department of Basic and Applied Science for Engineering, Via Scarpa 16, 00161 Roma, Italy*

**Short abstract:** Heat transfer can differ distinctly at the nanoscale from that at the macroscale. Recent advancement in experimental techniques has enabled a large number of interesting observations and understanding of heat transfer processes at the nanoscale.

In this summary we review recent advances in the methodology of Photoacoustic and Photothermal techniques. In particular we applied photoacoustic spectroscopy (PAS) to detect circular dichroism of intrinsic chiral materials [1] as well as extrinsic chiral metasurfaces [2-4].

In disordered media PAS is confirmed to be the most appropriate technique to determine separately the absorption and the scattering coefficients allowing to determine the size of both metallic (AgNP) [5], or semiconductor nanospheres (ZnO) [6, 7], or clusters of nanospheres bridged by the ligands [8], in contrast to nanolayered samples [9] or self-organized eutectic composites [10, 11].

On the other hand photothermal deflection spectroscopy (PDS) may be used as a complementary technique to measure the absorbance spectrum in nanostructures so to detect absorption lines, or photonic band gap in photonic crystals [12, 13], or to measure the out-of/in-plane thermal diffusivity in 2D materials [14].

We also underline some applications of photothermal radiometry (PTR) used to localize the internal heat sources where the pump light is absorbed, and to measure the effective thermal diffusivity. The modulation frequency obtained by an acousto-optical modulator ranges from 1 Hz up to 100 kHz, allowing the improvement of the thermal resolution till submicron range. We have applied PTR and IR Thermography techniques to PCM-VO<sub>2</sub> nanolayered samples [15-17], nanodisks [18] and W-doped VO<sub>2</sub> thin films [19, 20]. Such a technique has been applied also to carbon nanotube film deposited onto a silicon substrate: in this case PTR allows to detect the thermal wave interference in the film and to measure the effective thermal diffusivity of the CNT, and the thermal resistance with the substrate [21]. Photothermal radiometry and thermography can be also used to measure the emissivity of nanostructured materials, nanoantennas and metasurfaces designed so to have specific directional emittance properties [22, 23]. The invited talk summarizes several research topics and recent works done in collaboration with many partners (Universities, Research Centres and European Centre of Excellence *Ensemble3*).

## References

- [1] A. Benedetti et al. Scientific Reports, **7**, 5257 (2017).
- [2] Petronijevic, E.; Cesca T.; Scian C.; Mattei G.; Li Voti, R.; Sibilial C.; Belardini A., Scientific Reports **14**, 17210 (2024)
- [3] Petronijevic E.; Cesca, T.; Scian, C.; Mattei, G.; Li Voti, R.; Sibilial, C.; Belardini, A, Nanoscale **16**, 16477 (2024)
- [4] Petronijević, E., Belardini, A., Leahu, G., Li Voti, R., Sibilial, C, Optical Materials Express **12**, 2724, (2022)
- [5] R. Li Voti, et al. Int J Thermophys, **36**, 342 (2015).
- [6] F.R. Lamasra et al., Nanotechnology **28**, 375704 (2017).
- [7] F.R. Lamasra et al, Int J Thermophys, **39**, 110, (2018).
- [8] R. Li Voti et al., Nanoscale Advances **3**, 4692 (2021).
- [9] Cesarini, G., Leahu, G., Grilli, M.L., Sytkova, A., Sibilial, C., Li Voti, R., Physica Status Solidi (C) **13**, 998 (2016).
- [10] P. Osewski et al. Adv. Optical Mater. 1901617 (2020).
- [11] E. Petronijevic, et al. Advanced Materials, **35**, 2206005 (2023)
- [12] R. Li Voti, G. Leahu, E. Petronijevic, A. Belardini, T. Cesca, C. Scian, G. Mattei, C. Sibilial, Applied Sciences, **12**, 1109, (2022).
- [13] G. Leahu et al., Adv. Optical Mater. 2100670 (2021).
- [14] C. Yao, et al., Advanced Functional Materials (2024) DOI 10.1002/adfm.202405235
- [15] T. Cesca, et al., Nanoscale **12**, 851 (2020).
- [16] R. Li Voti, G. L. Leahu, M. C. Larciprete, C. Sibilial, M. Bertolotti, Int J Thermophys, **36**, 1004 (2015).
- [17] R. Li Voti et al. International Journal of Thermal Sciences **197**, 108832 (2024)
- [18] Emilija Petronijevic et al. Scientific Reports **14**, 25324 (2024)
- [19] A.Bile et al. Optical Materials **154**, 115732 (2024)
- [20] Maria Cristina Larciprete et al., APL Mater. **11**, 091107 (2023)
- [21] G. Leahu, R. Li Voti, M. C. Larciprete, C. Sibilial, M. Bertolotti, I. Nefedov, I. V. Anoshkin, Int J Thermophys, **36**, 1349 (2015).
- [22] M. Centini, M.C. Larciprete, R. Li Voti, M.Bertolotti, C.Sibilial, and M.Anteza, Opt. Express **28**, 19334 (2020).
- [23] M. Centini, A. Benedetti, M. C. Larciprete, A. Belardini, R. Li Voti, M. Bertolotti, and C. Sibilial, Phys. Rev. B, **92**, 205411 (2015).

# Mid-IR photothermal spectroscopy for liquid sensing

Bernhard Lendl<sup>1</sup>, Gustavo V. B. Lukasiewicz<sup>1,2</sup>, Daniela Tomasetig<sup>1</sup>, Savda Sam<sup>1</sup>, Jesus Hernan Mendoza Castro<sup>1</sup>, Dominik Kau-Wacht<sup>1</sup>, Liam O'Faolain<sup>3</sup>, Georg Ramer<sup>1,4</sup>, Nelson G. C. Astrath<sup>1</sup>

1. TU Wien, Getreidemarkt 9, 1060 Vienna (Austria)

2. Universidade Tecnológica Federal do Paraná, Medianeira, PR 85722-332 (Brazil)

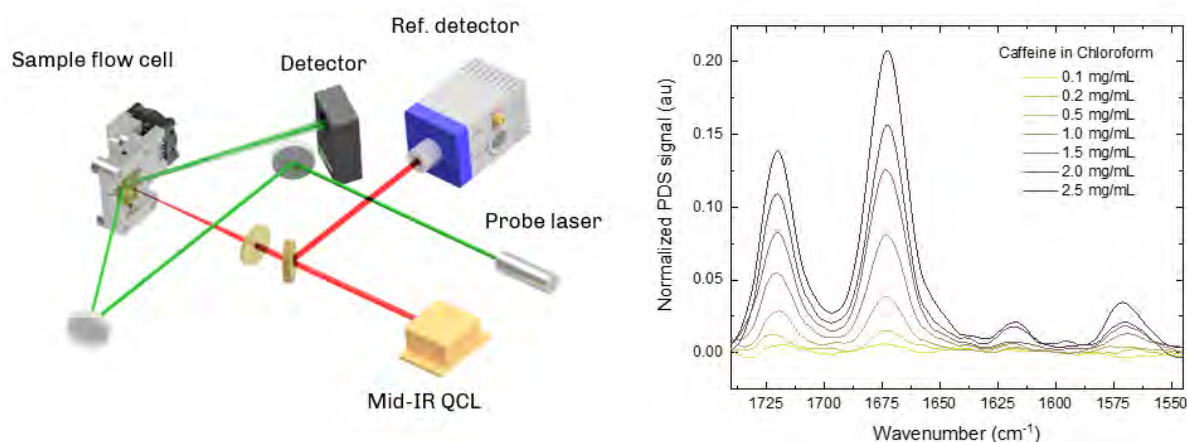
3. Munster Technological University, Cork, T12P928 (Ireland)

4. Christian Doppler Laboratory for Advanced Mid-Infrared Laser Spectroscopy in (Bio-)process Analytics, TU Wien, Vienna, 1060 (Austria)

5. Universidade Estadual de Maringá, Maringá, PR 87020-900 (Brazil)

**Short abstract:** Broadly tunable pulsed Mid-IR EC-QCL are used for direct quantitative measurement of solutes in liquids. In photothermal (PT) spectroscopy absorption induced local heating is detected using a second, visible laser. Different sensing modalities like PT lens, PT mirror and PT beam deflection will be discussed and selected examples presented.

After a review of the basic signal generation processes in photothermal spectroscopy different experimental realizations will be presented. These will include bench-top set-ups for photothermal lens (PTL), photothermal mirror (PTM) and photothermal beam deflection (PTD) spectroscopies. It has been found that quantitative analysis of strongly absorbing molecules such as water in weakly absorbing solvents such as chloroform is straight forward allowing for trace analysis. On the other hand, when dealing with strongly absorbing solvents quantitative analysis is only possible when using a phase resolved detection approach. The recorded PT spectra are compared with FTIR reference spectra showing an excellent agreement of the different measurement approaches. Quantitative measurements will be shown using water and caffeine as test analytes. Exemplarily Fig. 1 depicts the optical configuration used for PTD spectroscopy and shows concentration dependent PTD spectra of caffeine in chloroform.



**Fig. 1** left: schematic of the experimental set-up used for photothermal beam deflection (PTD) spectroscopy. Right: PTD spectra of caffeine in chloroform.

Furthermore, strategies for realizing an in-line probe for use in process analytical technology (PAT) settings and based on photothermal spectroscopy will be discussed in comparison with established mid-IR fiber optic probes based on attenuated total reflection measurement. The presentation will conclude reporting on most recent findings using an asymmetric Mach Zehnder Interferometer or ring resonators realized in SiN as sensitive transducers of refractive index changes which occur in PT spectroscopy of liquids.

# Integrated Photothermal Spectroscopy Systems: A Path Toward Mass Production using Semiconductor Processes

Maria V. Kotlyar<sup>1,2</sup>, Jenitta J. Mapranathukaran<sup>1,2</sup>, Gabriele Biagi<sup>1,2</sup>, Giulia Malvicini<sup>1,3</sup>,  
Bernhard Lendl<sup>3</sup> and Liam O’Faolain<sup>1,2</sup>

*1. Centre for Advanced Photonics and Process Analysis, Munster Technological University, T12 T66T, Cork, Ireland*

*2. Tyndall National Institute, T12 PX46, Cork, Ireland*

*3. Institute of Chemical Technologies and Analytics, TU Wien, Getreidemarkt 9/164, Vienna, 1060, Austria*

**Short abstract:** We demonstrate scalable photothermal spectroscopy using CMOS-compatible micro-ring resonators and wafer-bonded Fabry–Perot cavities, showing a potential route to mass manufacturable gas sensors through standard semiconductor fabrication techniques.

Photothermal spectroscopy (PTS) is gaining traction as a non-destructive, non-contact technique for trace gas detection, owing to its high sensitivity and strong potential for miniaturization [1]. In this work, we present two novel photonic device platforms that implement PTS using advanced microfabricated structures: silicon nitride micro-ring resonators (MRRs) [2] and wafer-bonded Fabry–Perot (FP) cavities incorporating integrated distributed Bragg reflectors (DBRs). Both platforms are fully compatible with semiconductor fabrication techniques, enabling scalable, cost-effective manufacturing and widespread deployment.

The first system is based on an integrated silicon nitride MRR that functions as a highly sensitive refractive index transducer. An excitation laser, tuned to a specific absorption line of the target analyte, induces localized heating in the surrounding medium. This thermal effect leads to a refractive index change, modulating the resonance condition of the MRR. A telecom-wavelength probe laser monitors the resonance shift, with 1-f and 2-f harmonic signals extracted to quantify the photothermal response [3]. The device is fabricated using CMOS-compatible processes—thermal oxidation, chemical vapor deposition, and electron beam lithography—offering a clear route to wafer-scale production. The chip can be assembled and packaged using standard photonic integration techniques.

The second demonstration employs wafer-bonded FP cavities formed by vertically stacking two DBR mirrors on a quartz substrate. These high-reflectivity mirrors are realized through alternating SiO<sub>2</sub>/Ta<sub>2</sub>O<sub>5</sub> layers. The cavity spacer, patterned in silicon using deep reactive ion etching (DRIE), defines the optical path length. Bonding is achieved via spin-coated benzocyclobutene (BCB), a process well-suited for high-throughput wafer-level packaging. The resulting FP sensors exhibit high optical finesse and are optimized for mid-infrared (mid-IR) operation, ideal for molecular fingerprinting in real-time gas sensing applications.

Though based on distinct optical architectures, both platforms offer viable paths toward compact, scalable, and high-performance PTS sensors. Their reliance on semiconductor microfabrication techniques—including wafer bonding and CMOS-compatible photonic integration—positions them for low-cost, large-scale production. These technologies hold strong promise for a wide range of applications, including environmental monitoring, industrial leak detection, and medical diagnostics, making them compelling candidates for next-generation integrated gas sensing solutions.

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## References

- [1] J.P. Waclawek, V.C. Bauer, H. Moser, and B. Lendl, “2f-wavelength modulation Fabry-Perot photothermal interferometry,” *Opt. Express* 24(25), 28958–28967 (2016).
- [2] M. V. Kotlyar, J.J. Mapranathukaran, G. Biagi, A. Walsh, B. Lendl, and L. O’Faolain, “Micro-Ring Resonator Assisted Photothermal Spectroscopy of Water Vapor,” *Sensors* 24(11), 24 (2024).
- [3] Hodgkinson, J.; Tatam, R.P. Optical gas sensing: A review. *Meas. Sci. Technol.*, 24, 12004 (2013).



# How to use a tunable laser and a gas filter cell for photoacoustic signal generation

Thomas Strahl<sup>1,2</sup>, Jonas Steinebrunner<sup>2</sup>, Eric Maier<sup>1,2</sup>, Johannes Herbst<sup>1</sup>, Sven Rademacher<sup>1</sup>,  
Jürgen Wöllenstein<sup>1,2</sup> and Katrin Schmitt<sup>1,2</sup>

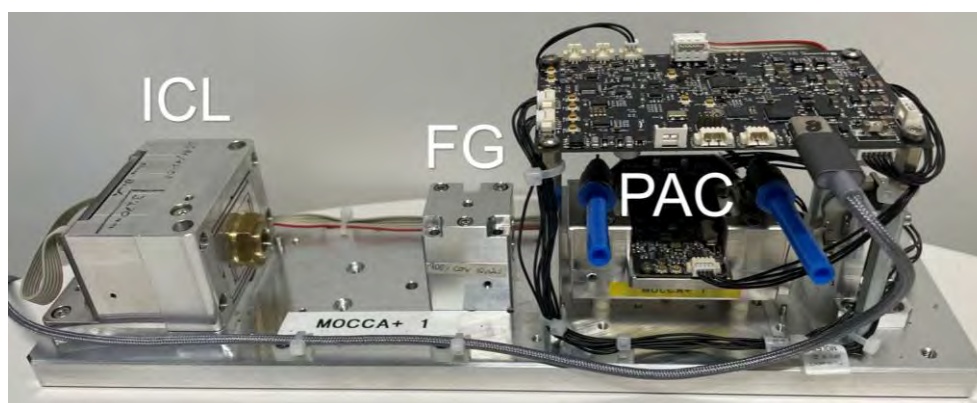
1. Fraunhofer Institute for Physical Measurement Techniques IPM, Gas and Process Technology Department, Georges-Köhler-Allee 301, 79110 Freiburg, Germany

2. University of Freiburg, Department of Microsystems Engineering—IMTEK, Laboratory for Gas Sensors, Georges-Köhler-Allee 102, 79110 Freiburg, Germany

**Short abstract:** A unique photoacoustic signal generation applicable for both single absorption lines and broad gas absorption is introduced which uses an intensity modulation realized through a minimal wavelength modulation of a typical tunable laser in combination with a gas filter cell.

In this work, a laser modulation concept for photoacoustic signal generation will be introduced and demonstrated. In the photoacoustic or photothermal spectroscopy (PAS and PTS) of gases, periodic modulation of light excites molecules (absorption) to generate photoacoustic (PA) or photothermal (PT) signals that consist of periodic pressure or temperature (or density) fluctuations. The generated signal correlates with the absorbed light intensity by the gas and allows a gas concentration determination [1,2].

The idea is that the light of a tunable laser will be passed through a gas filter cell before reaching the PA or PT detection module. The filter gas cell serves as a realization of a spectrally narrow optical notch filter, allowing suitable laser light at a specific wavelength to be ideally fully absorbed, while the laser light fully transmitted has a minimal wavelength variation. Technically, this intensity modulation (IM) can be realized through wavelength modulation (WM) in combination with a filter gas (FG). Of course, the tunable laser and filter gas cell needs to be chosen according to the absorption characteristics of the target gas. In principle, this modulation concept allows to address the light absorption by molecules with a single absorption lines or broad gas absorption in a specific wavelength range. The concept is demonstrated for methane as a small molecule with narrow or single line like absorption and toluene as large molecule (hydrocarbon) with a spectrally broad (or flat) absorption in the mid-infrared around  $3,27\text{ }\mu\text{m}$  ( $3057,7\text{ cm}^{-1}$ ). A tunable interband cascade laser (ICL) with an optical power of 8.5 mW is passed through a FG cell before reaching a resonant photoacoustic cell (dumbbell) as gas measurement cell (see Fig. 1). The FG cell of 1,5 cm length is filled with methane at a pressure of 10 mbar. This innovative concept allows a sensitive trace gas measurement with a detection limit below 10 ppb methane and 250 ppb toluene in nitrogen.



**Fig. 1:** Setup including interband cascade laser (ICL), filter gas cell (FG) and photoacoustic cell (PAC).

Since the initial signal generation of PTS is practically identical to PAS, as mentioned above, the demonstrated concept can likely be transferred to PTS. Furthermore, this new concept can be adopted to numerous target gases and applications including complex gas mixtures. An application-tailored combination of tunable lasers and filter gas cells can provide a path to unique gas sensing capabilities in terms of sensitivity and selectivity.

## References

- [1] Schilt, Stéphane, and Luc Thévenaz. "Wavelength modulation photoacoustic spectroscopy: Theoretical description and experimental results." *Infrared physics & technology* 48.2 (2006): 154-162.
- [2] Pinto, Davide, et al. "Parts-per-billion detection of carbon monoxide: A comparison between quartz-enhanced photoacoustic and photothermal spectroscopy." *Photoacoustics* 22 (2021): 100244.

# Towards Photonic Integration: Trace Gas Sensing by Balanced-Detection Interferometric Cavity-Assisted Photothermal Spectroscopy (ICAPS)

Johannes P. Waclawek<sup>1</sup>, H. Moser<sup>1</sup>, Ahmed Mahrous<sup>2,3,4</sup>, Mazen Erfan<sup>3,4</sup>, Tarik Bourouina<sup>2</sup>, and Bernhard Lendl<sup>1</sup>

1. TU Wien – Vienna University of Technology, 1060 Wien, Austria

2. ESYCOM Lab, Univ Gustave Eiffel, CNRS, F-77454 Marne-la-Vallée, France

3. Si-Ware Systems SAS, 16 rue Portalis, 75008 Paris, France

4. Faculty of Engineering, Ain-Shams University, 1 Elsarayat St., 11535 Abbaseya, Cairo, Egypt

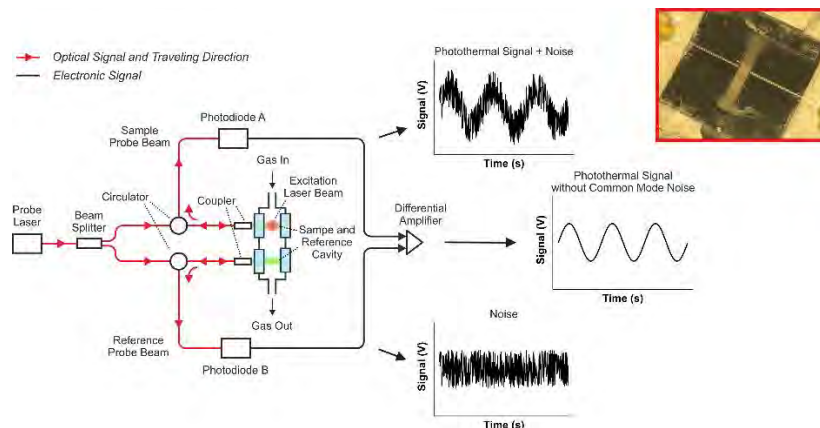
**Short abstract:** Compact gas sensing employing balanced-detection ICAPS is reported. Signal balancing was realized by using two identical cavities with a path length of only 1 mm, enabling efficient noise reduction. Latest results and progress towards sensor miniaturization, leveraging photonically integrated Fabry-Perot interferometers on silicon will be presented.

The miniaturization of sensitive as well as selective laser-based gas detectors is of big request among different fields of activity due to specific characteristics such as a fast sensor response or simply a small footprint. However, it still remains challenging. While methods based on direct absorption spectroscopy show a limited potential for miniaturization due to their dependence of sensitivity on the optical path length according to the Lambert-Beer law, indirect spectroscopic techniques of photothermal nature inherently exhibit high miniaturization potential, even down to integration onto a chip.

The *Interferometric Cavity-Assisted Photothermal Spectroscopy (ICAPS)* method has been proven highly suitable for sensitive and compact gas detection by application of a Fabry-Perot interferometer (FPI) as transducer for photothermal spectroscopy. The implementation of a balanced detection scheme to our developed system is a key improvement, which enhances the sensor's performance by efficient cancellation of noise (Fig. 1).

Within the presentation, recent results of a setup employing individual interferometers will be shown. Here, balanced-detection was realized by using two identical cavities having a path length of 1 mm and a total sample gas volume of a few mm<sup>3</sup>. The system uses an all fiber-coupled probe laser configuration, which detected the reflectance of the interferometers, enabling sensor operation close to the fundamental limit of shot noise. The metrological figures of merit were investigated by detection of different trace gases such as SO<sub>2</sub>, CO and NO using QCLs as powerful mid-infrared excitation sources. The induced refractive index changes were monitored by a near-infrared probe laser. For the targeted molecules a minimum detection limit down to the sub-ppbv level was achieved with a 1s integration time, corresponding to a normalized noise equivalent absorption of the order of  $10^{-9} \text{ cm}^{-1} \text{ W Hz}^{-1/2}$ .

Additionally, latest progress regarding sensor miniaturization will be discussed. FPIs made solely from single-crystalline silicon with Bragg mirrors consisting of silicon-air dielectric multilayers [2] were designed and fabricated. The FPIs allow easy coupling of the near-infrared beam by optical fibers positioned in the chip along aligned grooves (inset Fig. 1). First demonstration of ICAPS gas sensing employing a silicon FPI will be shown.



**Fig. 1.** Principle of balanced-detection ICAPS monitoring the interferometers reflectance [1]. Inset: Photograph of a designed and fabricated fiber-coupled photonic integrated interferometer having a mirror spacing of 1 mm.

## References

- [1] J. P. Waclawek, H. Moser, and B. Lendl, "Balanced-detection interferometric cavity-assisted photothermal spectroscopy employing an all-fiber-coupled probe laser configuration," *Opt. Express* 29, 7794-7808 (2021).
- [2] M. Malak Karam, et al., "Micromachined Fabry-Perot resonator combining submillimeter cavity length and high quality factor", *Appl. Phys. Lett.*, 21 (98), id. 211113 (2011).

# Bio-medical Applications - Sponsored by Project Brief



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# Laser-spectroscopic non-invasive glucose monitoring

Markus W. Sigrist<sup>1</sup> and Julien M. Rey<sup>2</sup>

1. ETH Zurich, Institute for Quantum Electronics, John-von-Neumann-Weg 9, CH-8093 Zurich (Switzerland)

2. University of Applied Sciences (ZHAW), Institute of Applied Mathematics and Physics, CH-8401 Winterthur (Switzerland)

**Short abstract:** Continuous non-invasive glucose sensing is of great interest. We present new results using two pulsed DFB-QCLs at pre-selected wavelengths and time-domain photoacoustic detection through the skin. Measurements performed on the middle finger at low and high glucose levels show a clear difference of the temporal decay of the PA signal.

Diabetes is a chronic metabolic disease which is increasing in incidence worldwide. Currently, it affects more than 400 million people globally. The normal glucose level for a healthy person under non-fasting conditions fluctuates during the day between ca. 60 and 130 mg/dL blood or 3.3 mmol/L – 7.15 mmol/L. There exist various methods or approaches to measure the blood glucose level either invasively (by collecting a droplet of blood with a needle) or minimally invasively (for continuous glucose monitoring in the interstitial fluid with a small filament within the skin, commercialized by companies such as Dexcom, Medtronic or Abbott). Great efforts are being put into the development of a totally non-invasive scheme [1-3]. Although highly desired, a reliable non-invasive technique is unfortunately still not established. In the past there have been various attempts to monitor the glucose level either in blood or in the interstitial tissue fluid with laser-spectroscopic schemes. Since Raman or near-IR spectroscopy have not proven successful so far for various reasons, the focus in recent times has moved to the mid-IR wavelength range. Glucose exhibits strong absorption peaks in the 8 to 11  $\mu\text{m}$  wavelength range without strong spectral interferences from lipids and other skin constituents (as in the near-IR), yet the penetration depth is limited to 0.1 mm due to strong water absorption, i.e. glucose can only be monitored in the interstitial fluid and not directly in the blood vessels.

Recent progress in non-invasive glucose detection has been reported using quantum cascade lasers (QCLs) in the mid-IR combined with photoacoustic spectroscopy [4,5] or with photothermal deflection spectroscopy as is currently pursued by the company DiaMonTech [6].

We started our non-invasive glucose monitoring with fiber-coupled QCLs operated at two pre-selected wavelengths (on-peak and off-peak of glucose absorption) and photoacoustic (PA) detection [7]. The home-made PA cell was in direct contact with the forearm of volunteers for continuous recording. The cell was continuously flushed with dry air to avoid enhanced humidity. An oral glucose tolerance test with healthy individuals and repeated blood glucose measurements every 10 minutes with a commercial (invasive) glucometer showed reasonable agreement with our continuous (non-invasive) PA measurements. A concentration uncertainty of  $\pm 30$  mg/dL at a confidence level of 90% was achieved without any data treatment. However, the sensitivity for the physiological range of glucose concentration, the overall stability as well as the reproducibility were still unsatisfactory. In a new approach we developed a time-domain PA setup with the aim to increase the *in vivo* reproducibility. Two pulsed QCLs at wavelengths of 1038  $\text{cm}^{-1}$  (on-peak) and 1195  $\text{cm}^{-1}$  (off-peak) are employed to generate PA signals that are recorded in the time domain. The ratio of these two PA signals is much less prone to acoustic signal fluctuations caused, e.g., by microphone responsivity drifts or by skin surface movements. Measurements performed on the middle finger at low (80 mg/dL) and high (158 mg/dL) glucose levels showed a clear difference of the temporal decay of the PA signal. The current reproducibility of  $\pm 24$  mg/dL for this time-domain scheme is similar to the previous results. However, these very first results prove the potential of this time-domain PA scheme presented here for *in vivo* non-invasive glucose sensing.

## References

- [1] W. V. Gonzales, A. T. Mobashsher, and A. Abbosh, “The Progress of Glucose Monitoring – A Review of Invasive to Minimally and Non-Invasive Techniques, Devices and Sensors,” *Sensors* **19**, 800 (2019)
- [2] D. Di Filippo, F.N. Sunstrum, J. U. Khan, and A.W. Welsh, “Non-Invasive Glucose Sensing Technologies and Products: A Comprehensive Review for Researchers and Clinicians,” *Sensors* **23**, 9130 (2023)
- [3] Z. Peng and Z. Yang, “Optical blood glucose non-invasive detection and its research progress,” *Analyst* **149**, 4830 (2024)
- [4] R. Kaysir, J. Song, S. Rassel, A. Aloraynan, and D. Ban, “Progress and Perspectives of Mid-Infrared Photoacoustic Spectroscopy for Non-Invasive Glucose Detection,” *Biosensors* **13**, 716 (2023)
- [5] R. Kaysir, T.M. Zaman, S. Rassel, J. Wang, and D. Ban, “Photoacoustic Resonators for Non-Invasive Blood Glucose Detection Through Photoacoustic Spectroscopy: A Systematic Review,” *Sensors* **24**, 6963 (2024)
- [6] T. Lubinski, B. Plotka, S. Janik, L. Canini, and W. Mäntele, “Evaluation of a Novel Noninvasive Blood Glucose Monitor Based on Mid-Infrared Quantum Cascade Laser Technology and Photothermal Detection,” *J. Diabetes Sci. Technol.* **15**, 6 (2021).
- [7] J. Kottmann, J.M. Rey, and M.W. Sigrist, “Mid-Infrared Photoacoustic Detection of Glucose in Human Skin: Towards Non-Invasive Diagnostics,” *Sensors* **16**, 1663 (2016)



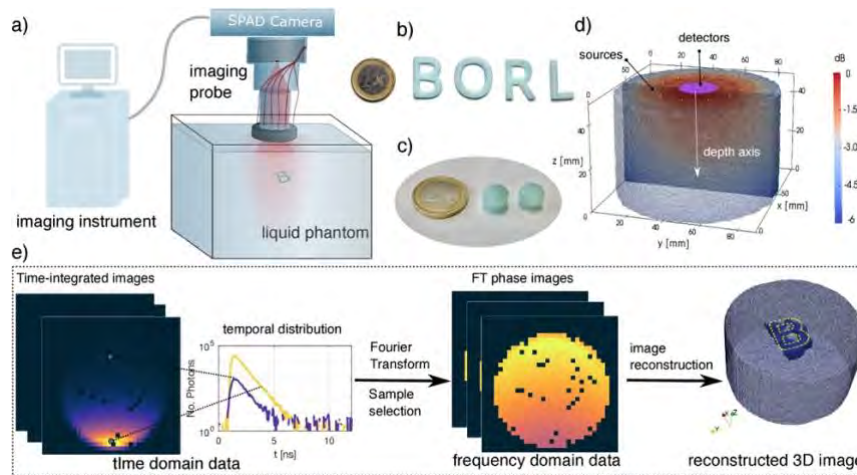
# Time domain near infrared spectroscopy and tomography for biomedical applications

Jingjing Jiang

Computational Optical Imaging Group, Biomedical Optics Research Laboratory, Department of Neonatology,  
University Hospital Zurich and University of Zurich

**Short abstract:** Near infrared spectroscopy (NIRS) measures chromophores in tissue using light at multiple wavelengths. We extended NIRS to 3D and developed a reflection-mode time-domain (TD) near infrared optical tomography (NIROT) system to image tissue oxygen saturation.

Near infrared spectroscopy uses light emitters and receivers at multiple wavelengths to measure the concentrations of various chromophores in biological tissues. For example, oxy- and deoxy-hemoglobin, which define an important physiological parameter - oxygen saturation, have characteristic absorption spectra. This is of great importance for many medical applications, e.g., the detection of hemorrhage and ischemia in preterm babies, and tumor hypoxia in cancer patients. The existence of optical window in near infrared region for biological tissue makes it possible to image deep tissue up to several centimeters. For this reason, we have developed a reflection-mode time-domain (TD) near infrared optical tomography (NIROT) system to image tissue oxygen saturation [1-3]. The system employs a super-continuum laser that emits picosecond light pulses with a broad spectrum at a high repetition rate. An acousto-optic tunable filter (AOTF) is used for selecting desired wavelengths to enable spectral measurements. After interacting with tissue, the reflected light with time-of-flight (ToF) information is captured by a single photon avalanche diode (SPAD) array sensor. This sensor has 32x32 pixels and each pixel captures ToF signals for 12.5 ns with time resolution of 48.8 ps. The dataset is sent to a workstation where image reconstructions are performed to generate 3D images. We have successfully tested the system in various tissue-mimicking phantom experiments and in-vivo studies [3,4] (Fig. 1). It has great potential for use in clinical environment.



**Fig. 1** (a) Schematic depiction of the liquid phantom setup with the TD NIROT. Photos of the (b) letter phantoms and (c) spherical inclusions and a 1-euro coin. (d) 3D view of the finite element model used for image reconstruction: sensitivity map of the phase component (Eq. (1)) for the sources (yellow dots) and selected detectors (purple dots). Note that the volume is a cylindrical model of. We made it smaller than the actual liquid phantom to speed up the image reconstruction. e) Temporal data processing and image reconstruction. 11 images of pixel with each pixel containing 256 time gates were obtained. We selected several pixels within the field of view and the temporal windows where the signal is above its noise level. Note that the dark spots in the images are hot pixels. The selected temporal distributions were transformed into frequency domain (FD) for the image reconstruction. The blue area marks the reconstructed inclusion, and the yellow dots indicate the ground-truth shape of the letter B.

## References

- [1] Jiang, J., Di Costanzo Mata, A., Lindner, et. al., Dynamic time domain near-infrared optical tomography based on a spad camera," Biomed. Opt. Express 11, 5470 (Oct 2020).
- [2] Jiang, J., Di Costanzo Mata, A., Lindner, et. al., A. Image reconstruction for novel time do- main near infrared optical tomography: towards clinical applications. Biomed. Opt. Express 11, 4723 (2020)
- [3] Jiang, J., Ackermann, M., Russomanno, et. al., Resolution and penetration depth of reflection-mode time-domain near infrared optical tomography using a ToF SPAD camera," Biomed. Opt. Express 13, 6711 (Dec 2022).
- [4] Jiang, J., Di Costanzo Mata, A., Ackermann, et al. (2024). Imaging Deep Haemorrhage and Ischaemia in Preterm Infants' Heads with Time-Domain Near-Infrared Optical Tomography: Phantom Study. 2023. Advances in Experimental Medicine and Biology, vol 1463. Springer, Cham.

# Towards tactile sensing by use of a flexible polymer foil with masklessly processed waveguides

Zhenyu Zhang<sup>1</sup>, Martin Angelmahr<sup>1</sup>, Ulrike Willer<sup>2</sup>, and Wolfgang Schade<sup>1,2</sup>

1. Fraunhofer Heinrich Hertz Institute, Fiber Optical Sensor Systems, Am Stollen 19H, 38640 Goslar (Germany)

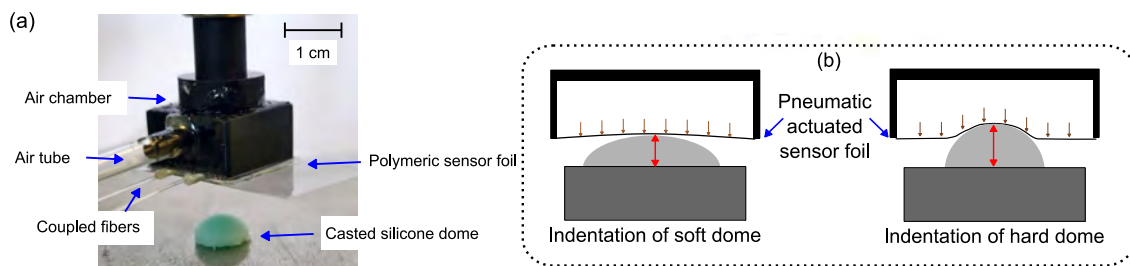
2. Clausthal University of Technology, EST, Am Stollen 19B, 38640 Goslar (Germany)

ulrike.willer@tu-clausthal.de

**Short abstract:** A flexible polymer foil with waveguide structure for the sensing of exerted force as well as sample properties such as surface structure or shore hardness is presented. The sensor mimics human tactile sense and is intended for application in minimal-invasive surgical invention and soft-robotics.

One of the great advances of human tactile sense is the ability to very sensitively distinguish areas of different stiffness or minute changes in pressure exerted by touching. While proximity sensors have been developed to, for example, control the approach of a robot towards a target [1], applications relying on tactile information are still scarce. This research concentrates on the development of a polymeric sensing foil that can be configured to sense stiffness, pressure or force and thus mimic palpation.

The sensor relies on measuring intensity changes of light transmitted through a polymeric waveguide that was processed by maskless photolithography using EpoCore on a flexible polymeric substrate [2]. Coupling to source and detector is done with polymeric optical fibers (POF). The foil is airtightly mounted over a cavity, thus forming an air chamber as depicted in figure 1 (a). With attached tubing, pressurized air can be led into the chamber, allowing the adjustment of a counter force and thus the adaption of the dynamic range for stiffness determination. If the application demands for it, the sensor could be further miniaturized.



**Fig. 1** (a) Photograph of the sensor device with polymeric sensor foil and connection to pressurized air and coupling POFs. One of the samples used for stiffness measurements is also depicted. (b) Sketch of the sensing principle for measuring the shore hardness: depending on the material properties and shape of the sample and the counterforce induced by the pneumatic actuation, a varying deformation of the foil occurs and thus different transmitted intensity is measured.

The basic principle of a stiffness measurement is sketched in figure 1(b) showing deformation of the sensor foil while pressed against samples of different stiffness. Silicone domes as depicted in figure 1 (a) with the same shape but different shore hardness were used as samples. Upon exertion of a force, both, the sample as well as the sensing foil, deform. The intensity of the light transmitted through the waveguide depends on the actual deformation of the foil. This however, is determined by the original shape of the sample and its deformation due to acting force, sample hardness and the pneumatic actuation of the foil. Dynamic change of the pneumatic actuation and scanning the sensor over the sample surface can mimic touching and palpation.

Examples of measuring forces exerted on the sensor foil as well as of sensing areas with different stiffness within a sample by scanning the surface will be presented as well as the reconstruction of the sample's surface structure by investigation of samples with different surface roughness.

By monitoring the changes in transmitted light intensity, the sensor achieved precise and reproduceable response for contact forces up to 5N. (with a minimal resolution of 0.1 N)

The work is carried out under grant agreement N°101092518 of the European Union's Horizon Europe programme.

## References

- [1] Dawood AB, Chavali VK, Mack T, Zhang Z, Godaba H, Angelmahr M and Althoefer K (2024) Abraded optical fibre-based dynamic range force sensor for tissue palpation. *Front. Robot. AI* 11:1489884. doi: 10.3389/frobt.2024.1489884
- [2] Zhang, Z.; Abdalwareth, A.; Flachenecker, G.; Angelmahr, M.; Schade, W. Polymer Waveguide Sensor Based on Evanescent Bragg Grating for Lab-on-a-Chip Applications. *Sensors* 2024, 24, 1234. <https://doi.org/10.3390/s24041234>

# Full-Domain 3D Digital Twin for SSAW Devices: Advancing Microfluidics and Sensing for One-Health

Felice Alberto Sfregola<sup>1</sup>, Annalisa Volpe<sup>1</sup>, Andrea Zifarelli<sup>1</sup>, Massimiliano Benetti<sup>2</sup>, Domenico Cannatà<sup>2</sup>, Vincenzo Spagnolo<sup>1,3</sup>, Pietro Patimisco<sup>1,3</sup>

1. Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, 70126 Bari, Italy

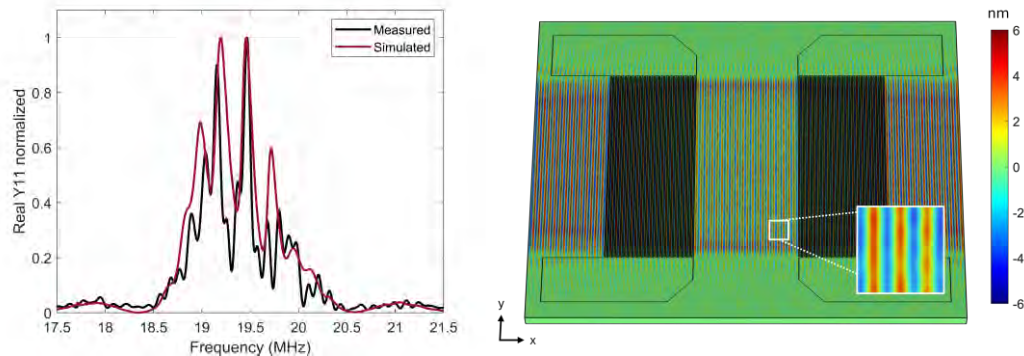
2. Institute of Microelectronics and Microsystems, IMM-CNR, Via del Fosso del Cavaliere 100, 00133 Rome, Italy

3. PolySense Innovations srl, Via Amendola 173, Bari 70126, Italy

**Short abstract:** A full-domain 3D digital twin of a LiNbO<sub>3</sub>-based Standing Surface Acoustic Wave (SSAW) device is developed and validated through impedance and interferometric measurements. The model reproduces both electrical and mechanical responses, including out-of-plane surface displacement patterns. This supports simulation-guided optimization of advanced lab-on-chip platforms for biosensing, particle and droplet manipulation in the framework of One-Health.

Precise manipulation of particles and fluids with Surface Acoustic Waves (SAWs) is pivotal in microfluidics and sensing applications, ranging from chemical detection [1] to biosensing in lab-on-chip devices [2]. The physics governing the SAW-based devices is inherently complex, involving the intricate interaction of multiple physical domains such as mechanics, piezoelectricity, acoustics, and fluid dynamics. Accurately modeling these phenomena demands advanced numerical methods capable of capturing wave propagation and electromechanical coupling with high precision.

This work develops a simulation-driven 3D digital twin of a SSAW device on 128° YX LiNbO<sub>3</sub>. It was developed in COMSOL Multiphysics using full-domain 3D modeling to capture complex electromechanical interactions. The model accurately replicated the device geometry, material properties, and boundary conditions, ensuring consistency with experimental conditions. Simulation studies included modal and frequency-domain analysis, together with time-domain simulations to capture transient phenomena during wave generation on the substrate. Validation was carried out through electrical response measurements with a Vector Network Analyzer (VNA) and out-of-plane displacement mapping using a Laser Doppler Vibrometer (LDV). The simulations closely matched experimental data, reliably predicting resonance properties (Fig. 1a) and surface displacement patterns (Fig. 1b). Moreover, the full-domain 3D digital twin allowed to study complex phenomena such as wave propagation, interference, and diffraction, usually challenging to analyze analytically due to the complexity of the physical interactions and the anisotropic properties of the LiNbO<sub>3</sub> substrate.



**Fig. 1** (a) Real part of the measured (black) and simulated (red) admittance. (b) Out-of-plane displacement for the full device under an AC signal corresponding to the experimental conditions. The inset provides a magnified view of alternating nodal and antinodal lines.

The validated digital twin enables predictive design of SAW-based devices, offering a systematic approach that replaces traditional trial-and-error approaches, thus speeding up the development of applications such as cell sorting and biomarker detection. Furthermore, the model provides a foundation for coupling structural and fluidic domains in acoustophoresis, enabling the study of acoustic forces acting on suspended particles and droplets within lab-on-a-chip systems.

## References

- [1] D.B. Go, M.Z. Atashbar, Z. Ramshani, and H.C. Chang, "Surface acoustic wave devices for chemical sensing and microfluidics: a review and perspective," *Analytical Methods* 9(28), 4112–4134 (2017).
- [2] J. Shi, D. Ahmed, X. Mao, S.C.S. Lin, A. Lawit, and T.J. Huang, "Acoustic tweezers: patterning cells and microparticles using standing surface acoustic waves (SSAW)," *Lab Chip* 9(20), 2890–2895 (2009).

# Interpretable EEG Analysis of Neurodegenerative Diseases for Precision Medicine Applications

Non-invasive neuro-imaging is rapidly expanding beyond traditional clinical settings, driven by compact, high-density sensor arrays and on-device artificial intelligence. Research into the application of deep learning (DL) models based on EEG signals is growing thanks to the increasing availability of large datasets, enabling end-to-end learning from raw inputs. Compared with convolutional and recurrent neural networks, Transformers have shown higher ability to deal with long-range dependencies and recognize patterns in sequential data, as well as employ more interpretable decision-making processes.

In this talk, we introduce an interpretable DL framework that leverages the self-attention mechanism of Transformer networks to analyse resting-state EEG in two neurodegenerative contexts, i.e., Alzheimer's Disease (AD) and Parkinson's Diseases (PD).

Specifically, the model is employed to distinguish healthy ageing from the prodromal phases in the AD spectrum, namely Subjective Cognitive Decline (SCD) and Mild Cognitive Impairment (MCI), using resting-state EEG signals [1][2].

Using the same architecture and minimal task-specific tuning, the pipeline is also exploited to classify Parkinson's patients from age-matched controls, achieving state-of-the-art performances on a large, multicentric public EEG dataset.

In both cases, the learned attention focuses on EEG biomarkers which are consistent with AD and PD pathophysiology. We demonstrate that classification confidence correlates with clinically-observed disease progression, opening a path toward longitudinal monitoring with wearable headsets in home or point-of-care environments.

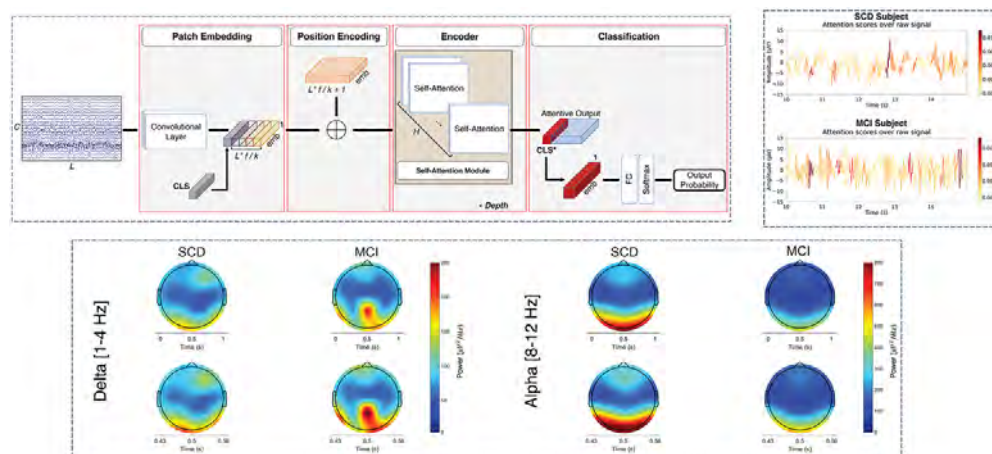


Fig. 1 Overall workflow of our interpretable EEG-Transformer.

## References

- [1] E. Sibilano\*, A. Brunetti\*, D. Buongiorno, M. Lassi, S. Micera, A. Mazzoni, V. Bevilacqua, "An Attention-Based Deep Learning Approach for the Classification of Subjective Cognitive Decline and Mild Cognitive Impairment using Resting-State EEG", *Journal of Neural Engineering*, vol. 20, art. no. 016048, 2023, doi: 10.1088/1741-2552/acb96e. \*Equal Contribution
- [2] E. Sibilano, D. Buongiorno, M. Lassi, A. Grippo, V. Bessi, S. Sorbi, A. Mazzoni, V. Bevilacqua, A. Brunetti, "Understanding the Role of Self-Attention in a Transformer model for the discrimination of SCD from MCI using resting-state EEG", *Journal of Biomedical and Health Informatics*, vol. 28, no. 6, pp. 3422-3433, June 2024, doi: 10.1109/JBHI.2024.3390606.



# Breath Analysis - Sponsored by Project D3- 4Health



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# Limits and prospects of infrared spectroscopy of breath for early diagnosis of asymptomatic diseases

**Kiran Sankar Maiti<sup>1</sup>, Susmita Roy<sup>2</sup>, Ronald Sroka<sup>3</sup>**

*1. TUM School of Natural Sciences, Department of Chemistry, Technical University of Munich, Lichtenbergstr. 4, Garching, 85747, Germany*

*2. Technical University of Munich, School of Medicine and Health, Department of Clinical Medicine, Klinikum rechts der Isar, Ismaninger Str. 22, 81675 Munich, Germany*

*3. Laser-Forschungslabor, LIFE-Center, LMU University Hospital, LMU Munich, 82152 Planegg, Germany*

Metabolites are byproducts of biochemical reactions within living cells, carrying crucial chemical information about cellular processes. Analyzing metabolites in biofluids such as blood, urine, and exhaled breath provides valuable insights into the body's internal chemistry and overall state[1]. With a reliable detection method, this approach could facilitate minimal- or non-invasive diagnostics, even for asymptomatic diseases.

Volatile metabolite-based diagnostics are particularly promising, as exhaled breath collection is entirely non-invasive. Infrared spectroscopy stands out as a powerful technique due to its non-destructive, label-free, and rapid molecular identification capabilities, making it superior to many existing methods[2]. However, significant challenges persist, including the high water vapor content in exhaled breath, which interferes with infrared measurements, and the complexity of distinguishing overlapping spectral features for accurate biomarker identification and quantification.

Despite these obstacles, advancements in sample preparation[3] and data analysis[4] have significantly improved infrared spectroscopy's diagnostic potential. The technique has already been successfully applied to detecting life-threatening diseases such as cancer, diabetes, cerebral palsy, and bacterial infections, achieving over 90% accuracy[5,6]. This presentation will highlight the advantages, challenges, and strategies to overcome these hurdles, paving the way for infrared spectroscopy to become a reliable future diagnostic tool for breath analysis[7].

## References:

- [1] K. S. Maiti, M. Lewton, E. Fill and A. Apolonskiy, "Human beings as islands of stability: Monitoring body states using breath profiles," *Sci. Rep.* 9:16167, 2019.
- [2] A. Apolonski, S. Roy, R. Lampe and K. S. Maiti "Molecular identification of bio-fluids in gas phase using infrared spectroscopy" *Applied Optics*, 59(17):E36, 2020.
- [3] K. S. Maiti, M. Lewton, E. Fill, and A. Apolonski, "Sensitive spectroscopic breath analysis by water condensation", *Journal of Breath Research* 12, 046003 (2018).
- [4] A. Apolonskiy and K. S. Maiti "Towards a standard operating procedure for revealing hidden volatile organic compounds in breath. The FTIR spectroscopy case. *Appl. Opt.* 60:4217, 2021
- [5] K. S. Maiti, E. Fill, F. Strittmatter, Y. Volz, R. Sroka, and A. Apolonski, "Towards reliable diagnostics of prostate cancer via breath" *Sci. Rep.* 11:18381, 2021.
- [6] K. S. Maiti "Non-invasive disease specific biomarker detection using infrared spectroscopy." *Molecules*. 28(5):2320, 2023
- [7] S. Roy, J. Hauer, and K. S. Maiti "Development of non-invasive diagnosis based on FTIR spectroscopy," *Vibrational Spectroscopy* 134:103724, 2024

# Photoacoustics for breath analysis: sources and setups

## Preliminary demonstration on cardiovascular diagnosis

Vicet Aurore, Seoudi Tarek, Abou Naoum Fadia, Ayache Diba, Pages Fanny, Rosenkrantz Eric,  
Gouzi Fares, Bahriz Michael.

1. IES, Univ. Montpellier, CNRS, F-34000 Montpellier, France

**Short abstract:** Spectroscopic breath analysis is a demanding application requiring high performances from the measurements systems. The variability of the subjects led to variabilities of the gas mixture that must be taken in consideration. We propose here a review of our works in infrared laser photoacoustic sensing applied to breath analysis.

Photoacoustic sensing relies on the detection of an acoustic wave generated by the modulated molecular absorption of light in a gaseous species. The soundwave can be detected by different techniques, using resonant or non-resonant transducers, in resonant or non-resonant acoustic cells configurations. Our group has been working on infrared antimonide lasers sources and on Quartz Enhanced Photoacoustic Spectroscopy (QEPAS) since several years on various molecule sensing [1]. We are now exploring innovating sensing techniques as well as out-of-lab applications and demonstrations.

Breath sensing is very demanding in terms of detection limits and experimental implementation. The gaseous mixture to analyze is composed of a warm, humid gas (high water vapor content), with high CO<sub>2</sub> concentration (up to 5%) that constitutes a challenge to overcome [2]. Within a collaboration with Montpellier University Hospital, we have identified four biomarkers and developed QEPAS demonstrators [3][4] combined to a spirometry setup (Ergocard from Medisoft company), dedicated to cardiovascular diseases exploration (Fig. 1). A measurement campaign was carried out during spring and summer 2024 with some patients and healthy volunteers. We will present the developments of the sensors, and the setup that was implemented during this campaign. We will discuss the preliminary results.

Eventually, we will expose our latest developments to improve our setups. These works address two directions: the first one aims to improve QEPAS sensing by coupling the sound wave to a multi-pass opto-acoustic cell, while the second one explores MEMS developments [5] and their application to photoacoustics.

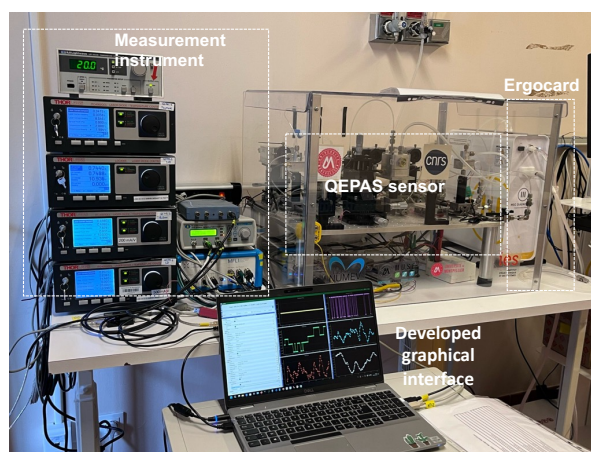


Figure 1. 4-gas QEPAS setup installed in Montpellier hospital for the clinical study.

## References

- [1] D. Ayache *et al.*, « Benzene sensing by Quartz Enhanced Photoacoustic Spectroscopy at 14.85  $\mu\text{m}$  », *Opt. Express*, vol. 30, n° 4, p. 5531, févr. 2022, doi: 10.1364/OE.447197.
- [2] J. Wojtas, Z. Bielecki, T. Stacewicz, J. Mikołajczyk, et M. Nowakowski, « Ultrasensitive laser spectroscopy for breath analysis », *Opto-Electron. Rev.*, vol. 20, n° 1, janv. 2012, doi: 10.2478/s11772-012-0011-4.
- [3] F. Gouzi, D. Ayache, C. Hédon, N. Molinari, et A. Vicet, « Breath acetone concentration: too heterogeneous to constitute a diagnosis or prognosis biomarker in heart failure? A systematic review and meta-analysis », *J. Breath Res.*, vol. 16, n° 1, p. 016001, janv. 2022, doi: 10.1088/1752-7163/ac356d.
- [4] N. Maurin *et al.*, « First clinical evaluation of a quartz enhanced photo-acoustic CO sensor for human breath analysis », *Sens. Actuators B Chem.*, vol. 319, p. 128247, sept. 2020, doi: 10.1016/j.snb.2020.128247.
- [5] T. Seoudi *et al.*, « Highly Sensitive Capacitive MEMS for Photoacoustic Gas Trace Detection », *Sensors*, vol. 23, n° 6, p. 3280, mars 2023, doi: 10.3390/s23063280.

# Diagnosis of colorectal cancer by the analysis of volatile organic compounds in the exhaled breath

Arcangelo Picciariello, MD, PhD, FEBS (Colo), FASCRS

1. Department of Experimental Medicine, University of Salento, Lecce, Italy

2. Department of Surgery, IRCCS "S. De Bellis", Castellana Grotte, Bari, Italy

**Short abstract:** Colorectal cancer is the second leading cause of death globally. Breath analysis of volatile organic compounds (VOCs) shows promise as an accurate, low-cost, and patient-friendly screening method. It can distinguish between healthy individuals, cancer patients, and those with precancerous polyps, making it a valuable tool for early diagnosis and prevention.

Colorectal cancer screening using the fecal occult blood test has proven to be lifesaving. However, it suffers from low patient compliance due to the unpleasantness of handling fecal samples and is further limited by unsatisfactory reliability. With the advent of precision medicine, there is now an opportunity to revolutionize colorectal cancer screening by developing new, reliable, cost-effective, and widely accepted screening tools. Recently, the analysis of molecular components in breath has been applied to the early diagnosis and monitoring of various diseases. This has given rise to a new branch of metabolomics known as "breathomics", which has been a focal point of research since Linus Pauling revealed a complex mixture of an estimated 250 VOCs in human breath.

Volatile organic compounds (VOCs) are produced during physiological and pathological processes. VOCs can also originate from exogenous sources such as food and drugs and microbiome metabolism. Once produced, VOCs are reversed into the bloodstream where they reach the pulmonary alveoli and are measurable in the exhaled breath[1,2]. While further validation through larger-scale studies is necessary, various investigations have already shown that patients with colorectal cancer exhibit a distinct pattern of VOCs in their exhaled breath compared to healthy individuals. This suggests that breath analysis could serve as a potential non-invasive diagnostic tool for detecting colorectal cancer.

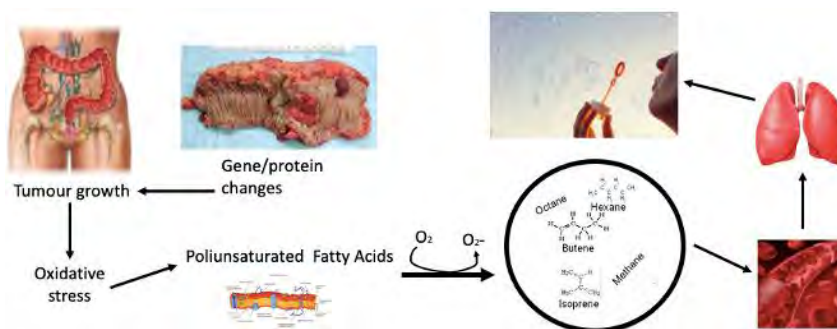


Fig. 1

## References

- [1] Altomare, D. F., A. Picciariello, M. T. Rotelli, M. De Fazio, A. Aresta, C. G. Zambonin, L. Vincenti, P. Trerotoli, and N. De Vietro. 2020. "Chemical signature of colorectal cancer: case-control study for profiling the breath print." *BJS Open* 4 (6):1189-99. doi: 10.1002/bjs5.50354.
- [2] Picciariello, A., A. Dezi, L. Vincenti, M. G. Spampinato, W. Zang, P. Riahi, J. Scott, R. Sharma, X. Fan, and D. F. Altomare. 2024. "Colorectal Cancer Diagnosis through Breath Test Using a Portable Breath Analyzer-Preliminary Data." *Sensors (Basel)* 24 (7). doi: 10.3390/s24072343.



# Quartz-Enhanced Photoacoustic Sensor for Real Time and In-line Detection of Methane in Exhaled Breath

Nicoletta Ardito<sup>1</sup>, Arianna Elefante<sup>2</sup>, Andrea Zifarelli<sup>1</sup>, Pietro Patimisco<sup>1</sup>, Marilena Giglio<sup>1</sup>, Vincenzo Spagnolo<sup>1</sup>, and Angelo Sampaolo<sup>1</sup>

1. PolySense Lab-Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari, Italy

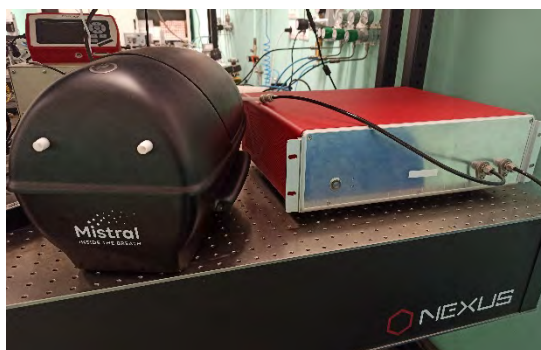
2. Institute for Photonics and Nanotechnologies (IFN), National Research Council, Via Amendola 173, Bari, Italy

**Short abstract:** We report on the development of a real-time breath analysis system combining an in-line breath sampler with a Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) sensor. Calibrated for methane detection, it achieves a detection limit of 175 part-per-billion, well below endogenous methane concentrations, providing high sensitivity and rapid response for non-invasive health diagnostics.

Breath analysis has emerged as a promising non-invasive technique for early disease detection and continuous health monitoring by targeting volatile organic compounds (VOCs) as biomarkers of physiological and pathological conditions [1]. Although gas chromatography–mass spectrometry (GC-MS) is regarded as the analytical gold standard for VOC identification due to its high sensitivity and molecular specificity, its bulky instrumentation, high cost, and lack of real-time operation significantly limit its applicability in decentralized or point-of-care applications.

Optical sensors based on laser absorption spectroscopy (LAS) offer a viable solution for VOCs detection, as many compounds exhibit strong and distinct absorption features in the mid-infrared region. Among these, Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) has gained considerable attention for trace gas detection [2]. QEPAS leverages the principles of Photoacoustic Spectroscopy (PAS), employing a Quartz Tuning Fork (QTF) as an acoustic transducer which converts laser-induced pressure waves into electrical signals via the piezoelectric effect of quartz [3].

In this work, we report the development and laboratory validation of a compact ICL-QEPAS sensor integrated in-line with the Mistral breath sampler (Predict Care Spa), enabling real-time and non-invasive analysis of exhaled breath. The Mistral device selectively collects the alveolar fraction enriched by pulmonary gas exchange, thereby reducing dilution from dead space air and enhancing the accuracy of the sampled biomarkers. The QEPAS sensor, coupled directly downstream, allows for rapid response and sensitive detection of target gas species. A picture of the developed experimental setup is shown in Fig. 1.



**Fig. 1** Picture of the developed QEPAS sensor system: on the left the Mistral sampler; on the right the compact QEPAS unit.

Tested for methane (CH<sub>4</sub>) detection, as a representative analyte due to its clinical relevance in metabolic and gastrointestinal disorders, the system was calibrated in dry/wet Nitrogen achieving a sensitivity of 0.80 mV/ppm and a minimum detection limit (MDL) of 175 part-per-billion, well below its typical endogenous concentrations, even with a signal integration time as short as 0.1 seconds [4]. Furthermore, validation tests were performed on human breath, demonstrating the system's applicability in real-world clinical settings.

## References

- [1] B. De Lacy Costello, A. Amann, H. Al-Kateb, C. Flynn, W. Filipiak, T. Khalid, D. Osborne, and N. M. Ratcliffe, "A review of the volatiles from the healthy human body," *J Breath Res* **8**, 014001 (2014).
- [2] A. Sampaolo, P. Patimisco, M. Giglio, A. Zifarelli, H. Wu, L. Dong, and V. Spagnolo, "Quartz-enhanced photoacoustic spectroscopy for multi-gas detection: A review," *Anal Chim Acta* **1202**, 338894 (2022).
- [3] P. Patimisco, A. Sampaolo, L. Dong, F. K. Tittel, and V. Spagnolo, "Recent advances in quartz enhanced photoacoustic sensing," *Appl Phys Rev* **5**, 17 (2018).
- [4] D. Roccarina, E. C. Lauritano, M. Gabrielli, F. Franceschi, V. Ojetti, and A. Gasbarrini, "The role of methane in intestinal diseases," *American Journal of Gastroenterology* **105**, 1250–1256 (2010).

# Development and Optimization of Photo-Acoustic sensors based on multi-pass QEPAS for medical applications

Fadia Abou Naoum, Fanny Pagès, Michael Bahriz, Aurore Vicet

*Institute of Electronics and Systems (IES) – Univ. of Montpellier – 34000 Montpellier (France)*

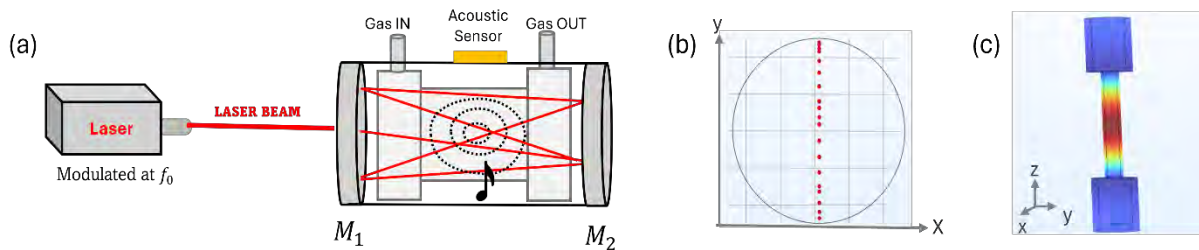
**Short abstract:** The basic principle of Photo-Acoustic measurement using an acoustic resonator is improved in this work by locally increasing the light density provided near the resonator to improve the limit of detection. To do so, the addition of a multi-pass optical cell to the acoustic setup is considered.

Despite advancements in air quality monitoring, concerns about indoor air pollution persist due to the lack of real-time and highly sensitive sensors capable of evaluating long exposure to hazardous gases and their health effects. Certain pollutants, such as carbon monoxide (CO) and volatile organic compounds (VOCs) like benzene and formaldehyde, often exceed regulatory guideline values indoors, posing significant health outcomes, including cardiovascular and cardiorespiratory diseases. This study, conducted in collaboration with medical doctors from Montpellier Hospital, aims to assess indoor air pollution using two complementary approaches. The first investigates the impact of chronic exposure to high pollutants amounts on cardiovascular system by analyzing exhaled breath in an animal model, while the second examines respiratory health effects under real-life conditions on human being. These strategies require the development of highly sensitive, real-time sensors, which we address through quartz-enhanced photoacoustic spectroscopy (QEPAS) [1].

QEPAS uses a modulated infrared laser source to spectrally scan the absorption line of the target gases. Unlike traditional PA approach that rely on microphones as transducer, QEPAS accumulates the acoustic energy in a sharply resonant quartz tuning fork (QTF) that acts as piezoelectric transducer with a very high-quality factor ( $\sim 8000$ ) making it immune to environmental acoustic noise.

For CO detection, we use a quantum cascade laser (QCL) emitting at  $4.7\text{ }\mu\text{m}$ , while benzene and formaldehyde detection rely on QCLs emitting at  $14.85\text{ }\mu\text{m}$  and  $5.6\text{ }\mu\text{m}$ , respectively. These mid-infrared wavelengths maximize absorption, achieving minimum detection limits (MDL) of 20 ppbv for CO [2] and 30 ppbv for benzene [3] within 1 second integration time.

To further enhance QEPAS sensitivity, we aim to develop a setup that combines an acoustic resonant cell with optical multipass. The initial focus is on designing and optimizing the acoustic resonant cell, which plays a crucial role in amplifying the PA signal. Once achieved, we will integrate the multipass optical cell, as illustrated in Fig. 1(a), to increase the optical path length through multiple reflections between highly reflective mirrors [4] before reaching the acoustic sensor. This approach significantly improves laser-gas interaction, leading to a lower MDL.



**Fig. 1** (a) Schematic of a PAS sensor with a multipass cell (MPC), (b) Simulated laser spot pattern generated using a theoretical model with two spherical mirrors, (c) Pressure (a.u.) in the first order acoustic mode of the acoustic cavity.

Acoustic simulations have been conducted using COMSOL Multiphysics to optimize a simple cylindrical resonant cell. These simulations evaluate the frequency response and pressure wave (Fig. 1(c)) distribution within the acoustic cavity to determine its resonance frequency. Additionally, numerical simulations based on ray propagation calculations have been performed to analyze the spot patterns inside the MPC (Fig. 1(b)). By optimizing mirror parameters and reflection angles, we aim to maximize the effective optical path.

## References

- [1] Kosterev, Anatoliy A., et al. "Quartz-enhanced photoacoustic spectroscopy." *Optics letters* 27.21 (2002): 1902-1904.
- [2] Maurin, Nicolas, et al. "First clinical evaluation of a quartz enhanced photo-acoustic CO sensor for human breath analysis." *Sensors and Actuators B: Chemical* 319 (2020): 128247.
- [3] Ayache D, Trzpil W, Rousseau R, Kinjalk K, Teissier R, Baranov AN, Bahriz M, Vicet A. "Benzene sensing by quartz enhanced photoacoustic spectroscopy at  $14.85\text{ }\mu\text{m}$ ." *Optics Express* 30.4 (2022): 5531-5539.
- [4] D. Herriott, H. Kogelnik, and R. Kompfner, "Off-axis paths in spherical mirror interferometers," *Appl. Opt.* 3, 523 (1964).

# IR-D34Health: A Strategic Research Infrastructure for the Future of Digital Healthcare

**Lorena Nappa<sup>1</sup>, Maria Teresa Pasqua<sup>1</sup>**

*1. D3-4Health Foundation, Viale Regina Elena 295, 00185 Roma, Italy*

**Short Abstract:** The IR-D34Health infrastructure, developed within the framework of the Italian PNC project Digital Driven Diagnostics, Prognostics and Therapeutics for Sustainable Healthcare (D34Health), represents a strategic ecosystem for accelerating innovation in the field of digital diagnostics and therapeutics. As part of the broader research initiative co-funding C-PASS 2025, this infrastructure is designed to support translational research through a network of highly specialized laboratories, enabling the integration of photonics, spectroscopy, and sensor technologies into clinical and biomedical applications.

IR-D34Health aims to facilitate interdisciplinary collaboration by bridging expertise across academia, healthcare institutions, and industry. It is expected to foster convergence among key research domains, including medical engineering, artificial intelligence, biophotonics, and health data science. A core mission of IR-D34Health is to redefine the concept of research training. Through shared access to advanced facilities and the implementation of dedicated educational programs, the infrastructure supports the development of innovative learning pathways and career trajectories. It promotes skill-building for young researchers and enhances collaboration across disciplines, nations, and sectors. By creating a dynamic, cross-sectoral environment, IR-D34Health contributes to the advancement of next-generation healthcare solutions and the development of a digitally enabled and globally connected research community.

# Quartz and Cantilever-Enhanced Photoacoustic Spectroscopy



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# Real time monitoring of N<sub>2</sub>O and CO emissions from vehicles using a Quartz-Enhanced Photoacoustic sensor

Patimisco P.<sup>1,2</sup>, Olivieri M.<sup>1</sup>, Zifarelli A.<sup>1</sup>, Sampaolo A.<sup>1,2</sup> and Spagnolo V.<sup>1,2</sup>

<sup>1</sup> PolySense Lab, Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari, 70126 Italy

<sup>2</sup> PolySense Innovations srl, Via Amendola 173, Bari, 70126 Italy

Greenhouse gases represent a crucial component of Earth's atmospheric system, playing a fundamental role in maintaining the planet's heat balance through their ability to absorb and emit infrared radiation. Anthropogenic activities have increased the atmospheric concentration of these gases, leading to enhanced global warming effects. The primary greenhouse gases include carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>), nitrous oxide (N<sub>2</sub>O), and water vapor (H<sub>2</sub>O). Among the other pollutants, carbon monoxide (CO) stands out as one of the most hazardous for human health. In urban areas, vehicle emissions represent the primary source of CO, produced through incomplete fuel combustion, with concentrations significantly higher than in unpolluted areas (~50 ppb). Furthermore, vehicles emissions, particularly from those equipped with catalytic converters, partially contribute to the global atmospheric N<sub>2</sub>O budget, whose atmospheric concentration is ~300 ppb. The deployment of portable and reliable sensors to monitor these emissions is crucial for understanding their sources, assessing their impact, and developing effective mitigation strategies.

Quartz Enhanced Photoacoustic Spectroscopy (QEPAS) sensors offer an effective solution for monitoring air pollutants, providing high selectivity and sensitivity, compact dimensions, and rapid response times. Photoacoustic (PAS) basic principle consists in detecting sound waves induced by gas non-radiative energy relaxation as consequence of infrared modulated light absorption. QEPAS represents an evolution of the PAS approach and exploits a quartz tuning fork (QTF) to transduce the acoustic wave into an electric signal. Mid-IR Quantum Cascade Lasers (QCLs) have been employed as light source in QEPAS-based sensor to target the absorption bands of both N<sub>2</sub>O and CO.

Here we report on the realization of a QEPAS-based system employing a QCL with a central emission wavelength at 4.61  $\mu\text{m}$  and a T-shaped QTF coupled with a pair of acoustic resonator tubes to amplify the sound wave. A ~1 min ramp was added to the fast laser modulation to scan the 2190.6-2188.7  $\text{cm}^{-1}$  spectral range, where well-resolved absorption features of N<sub>2</sub>O and CO were selected. Laboratory calibrations with certified gas cylinders demonstrated the sensor's ability to detect N<sub>2</sub>O and CO at hundreds and tens of ppb level, respectively, at a working pressure of 300 Torr and an integration time of 100 ms. We demonstrated the sensor capability to continuously monitor the QEPAS signal of the two gases both in indoor and outdoor environments. Indoor measurements were carried out over several days by sampling air inside the laboratory, while outdoor measurements took place in a university parking area in Bari to continuously monitor vehicle emissions. During spectral scans, the laser power, the sample temperature and its water vapor content was continuously measured, to eventually compensate for their influence on QEPAS signal. The resulting performances demonstrated its applicability for the realization of a compact and portable sensor for emission monitoring in urban areas.



# QEPAS Analyzer for Solids and Liquids

Judith Falkhofen<sup>1,2</sup>, Marcus Wolff<sup>1</sup>

1. Hamburg University of Applied Sciences, Berliner Tor 21, 20099 Hamburg, Germany

2. University of the West of Scotland, High Street, Paisley PA1 2BE, Scotland, UK

**Short abstract:** Quartz-enhanced photoacoustic spectroscopy (QEPAS) employs a quartz tuning fork (QTF) as detector for the photoacoustic signal and enables laser spectroscopic gas sensors with extraordinarily high detection sensitivity [1]. We adapted this powerful technique for the analysis of solid and liquid samples and present potential applications and newest results.

Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) is a technique in which the soundwave is detected by a quartz tuning fork (QTF). It enables particularly high specificity with respect to the excitation frequency and is well known for an extraordinarily sensitive analysis of gaseous samples. So far, this technique has almost exclusively been used for the investigation of gaseous samples. The most common setup is the so called on-beam configuration. This involves the light passing through the gap between the prongs of the QTF. To amplify the signal, the QTF is often positioned between two identical cylindrical resonance tubes. In the off-beam configuration, the sound pressure wave is detected at a certain distance from the laser beam. The QTF is here typically positioned outside a resonance tube at a narrow opening [1-4].

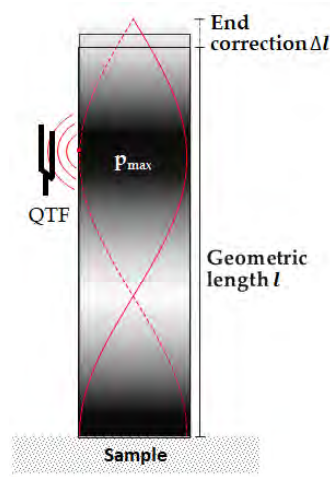


Fig. 1 Sound pressure amplitude in the half-open cell.

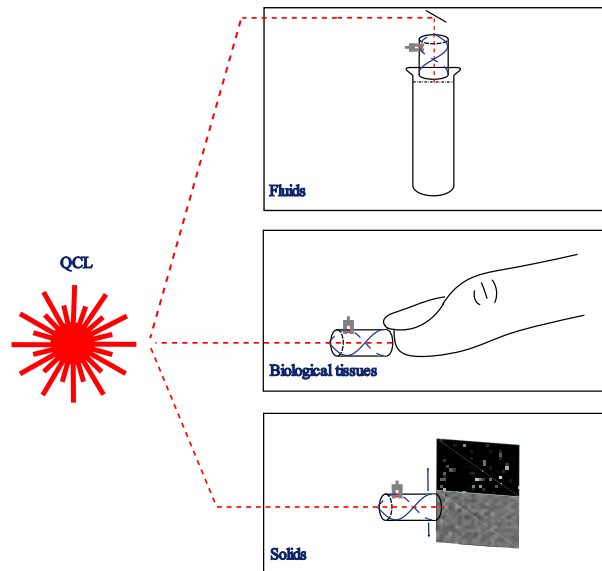


Fig. 2 Potential applications of the QEPAS sensor for solids and liquids.

We have developed a photoacoustic (PA) cell that allows it to apply this powerful technique for the analysis of solid and liquid samples. The cell represents a half-open cylinder that exhibits an acoustical resonance frequency equal to that of the QTF and, therefore, additionally amplifies the PA signal [5-7]. The antinode of the sound pressure of the first longitudinal overtone can be accessed by the sound detector (see Figure 1). We present newest experimental results and potential applications, reaching from medical diagnostics to imaging (see Figure 2).

## References

- [1] B. Li, G. Menduni, M. Giglio, P. Patimisco, A. Sampao, A. Zifarelli, H. Wu, T. Wei, V. Spagnolo, L. Dong, „Quartz-enhanced photoacoustic spectroscopy (QEPAS) and Beat Frequency-QEPAS techniques for air pollutants detection: A comparison in terms of sensitivity and acquisition time”, *Photoacoustics* **31**, 100479 (2023).
- [2] S. Angstenberger et al., "Coherent control in quartz-enhanced photoacoustics: fingerprinting a trace gas at ppm-level within seconds", *Optica* **12.1**, 1-4 (2025).
- [3] M. Yang et al. "Highly sensitive QEPAS sensor for sub-ppb N<sub>2</sub>O detection using a compact butterfly-packaged quantum cascade laser", *Applied Physics B* **130.1**, 6 (2024).
- [4] T. Liang et al. "High-sensitivity methane detection based on QEPAS and H-QEPAS technologies combined with a self-designed 8.7 kHz quartz tuning fork", *Photoacoustics* **36**, 100592 (2024).
- [5] J. Falkhofen, B. Baumann, M. Wolff, "New Photoacoustic Cell Design for Solid Samples", *Eng. Proc.* **58**, 86 (2023).
- [6] J. Falkhofen, M.-S. Bahr, M. Wolff, "Quartz Enhanced Photoacoustic Spectroscopy on Solid Samples", *Sensors* **24**, 4085 (2024).
- [7] J. Falkhofen, M. Wolff, "Calibration of a Quartz Tuning Fork as a Sound Detector", *Appl. Sci.* **15**, 3655 (2025).

# PPB-level Detection of Methane using Dielectric Coated Side-polished Fibers with Quartz-enhanced Photoacoustic Spectroscopy

Cian F. Twomey<sup>1</sup>, Gabriele Biagi<sup>1</sup>, Albert A. Ruth<sup>2</sup>, Farhan Ali<sup>3</sup>, Andrea Di Falco<sup>3</sup>, Liam O'Faolain<sup>1,4</sup>,  
(the late) Anton J. Walsh<sup>1,4</sup>

1. Centre for Advanced Photonics and Process Analysis, Munster Technological University, Cork, T12 P928, Ireland

2. School of Physics and Environmental Research Institute, University College Cork, Cork, Ireland

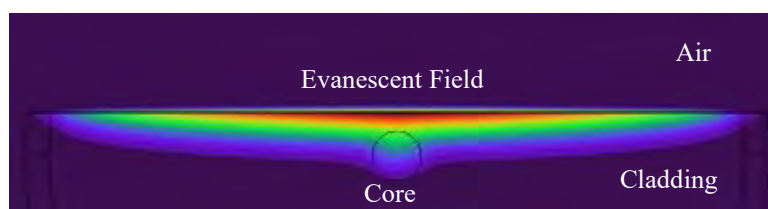
3. School of Physics and Astronomy, University of St Andrews, St Andrews, Fife, KY16 9AJ, Scotland

4. Tyndall National Institute, Lee Maltings Complex Dyke Parade, Cork, T12 R5CP, Ireland

**Short abstract:** We present an all-fiber-based evanescent wave laser gas analyzer using quartz-enhanced photoacoustic spectroscopy using a dielectric-coated side-polished fiber, custom quartz tuning fork, and acoustic micro-resonators. The coating enhances the air-confinement factor of the SPF to several percent, enabling trace gas detection in parts per billion as demonstrated with methane.

Most QEPAS sensor configurations use free-space optics and a focused laser beam as the excitation source. These free-space optics are susceptible to misalignment over time and if the beam touches the inside of the tubes it will induce thermal noise. This low misalignment tolerance limits their effectiveness and use in harsh environments such as agricultural or industrial settings. Laser gas sensors such as QEPAS sensors can be made more durable and robust by confining the light within optical fibers or silicon photonic waveguides and using evanescent waves (EW) as the optical excitation source.

Using the EW to interact with the sample analyte is a promising approach to avoid the need for sensitive alignment. For optical fibers, side-polishing [1] is a common technique to provide analyte access to the EW. The fibers used were Corning SM-28 fibers which were polished down to within a few microns of the core and had a 17 mm polished section. At the polished surface of the fiber, EW constitutes only a small fraction of the total mode power. Using the EW from a regular side-polished fiber (SPF) with QEPAS, it was demonstrated that 34 ppmv of methane could be detected with a 300 ms accumulation time [2]. To enhance the sensitivity of the EW-QEPAS sensor, we simulated and experimentally tested different dielectric coatings applied to the surface of the SPF. These dielectric materials, having a refractive index higher than the remaining cladding thickness, redirect more light toward the dielectric film surface, increasing the EW intensity to several percent. To confirm this enhancement, we measured methane (CH<sub>4</sub>) using both uncoated SPFs and those coated with dielectric films of varying thicknesses. The SPFs used in this study were coated with zirconium dioxide (ZrO<sub>2</sub>) layers ranging from 130 to 200 nm, with thickness values determined through COMSOL simulations. At 1653.7 nm, the absorption wavelength of methane used in this study, the refractive index of the ZrO<sub>2</sub> was 1.8531. Experimentally, we saw a 42x QEPAS signal enhancement using a 170 nm zirconia coating (air-confinement factor of 0.16%). With an air-confinement factor of over 3.5% parts per billion level methane detection with optical fiber is made possible using the EW of a coated SPF. The air-confinement factor can be improved to ~7% by using a ZrO<sub>2</sub> coating with a thickness close to 200 nm. The dielectric coating thickness can be engineered to enhance the EW of any desired wavelength that is within the transparency window of the SMF-28 fibers. In conclusion, covering an SPF with a high refractive index coating enhanced the evanescent field and led to a strong photoacoustic effect in methane. The stronger evanescent field leads to a significant enhancement in the QEPAS signal while maintaining the advantages of fiber-based excitation.



**Fig. 1** Mode profile of a zirconia-coated side-polished fiber.

## References

- [1] L. Zhuo, J. Tang, W. Zhu, H. Zheng, H. Guan, H. Lu, Y. Chen, Y. Luo, J. Zhang, Y. Zhong, J. Yu, Z. Chen, Side Polished Fiber: A Versatile Platform for Compact Fiber Devices and Sensors, *Photonic Sensors* 13 (2023) 230120. doi:<https://doi.org/10.1007/s13320-022-0661-x>.
- [2] C. F. Twomey, G. Biagi, A. A. Ruth, M. Giglio, V. Spagnolo, L. O'Faolain, A. J. Walsh, Evanescent wave quartz-enhanced photoacoustic spectroscopy employing a side-polished fiber for methanesensing, *Photoacoustics* 36 (2024) 100586. doi:<https://doi.org/10.1016/j.pacs.2024.100586>.

# Implementation and calibration of an in-situ sensor for isotopic monitoring of atmospheric CO<sub>2</sub> based on QEPAS

Yuliy Moreno-Sanoyan<sup>1</sup>, Marcos Martín-Romo<sup>1</sup>, Oscar E. Bonilla-Marique<sup>1</sup>, Aida Domínguez-Sáez<sup>2</sup>,  
Manuel Pujadas<sup>2</sup>, Marta Ruiz-Llata<sup>1</sup>

1. Universidad Carlos III de Madrid (UC3M), C/ Butarque 15, 28911 Leganés (Spain)

2. Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), 28040 Madrid (Spain)

**Short abstract:** We have developed a gas analyzer for precise measurement of carbon dioxide main isotopologues (<sup>12</sup>CO<sub>2</sub> and <sup>13</sup>CO<sub>2</sub>) based on the Quartz Enhanced Photoacoustic Spectroscopy (QEPAS) technique. We report on sensor performance and on the QEPAS signal model we have designed to fit and extract the concentration parameters.

Quartz Enhanced Photoacoustic Spectroscopy technique [1] combines the high sensitivity and specificity characteristics of other spectroscopy techniques with the advantage of requiring a small volume of sampled air, which gives it great potential for field deployment for atmospheric measurements [2]. In this work, a prototype QEPAS analyzer has been developed for the in-situ measurement of atmospheric CO<sub>2</sub>. For its implementation, core components are commercially available: acoustic detection module (ADM01, Thorlabs), quantum cascade laser (L12004-2310H-E, Hamamatsu) and data acquisition board (NI-USB-6361, National Instruments). The sensor operates in an area of the spectrum in which absorption peaks of the two main carbon isotopes that form the molecule of this gas are identified, so we investigate its application to determine the isotopic ratio  $\delta^{13}\text{C}$ .

The QEPAS sensor has been characterized in the laboratory using a bottle of CO<sub>2</sub> with unknown isotope ratio (but constant for all measurements) by diluting its concentration from 5000 ppm to 100 ppm. Measurements at the same concentrations have also been performed using a bottle of single isotope <sup>13</sup>CO<sub>2</sub>. The results obtained show a perfect linear relationship between the gas concentration and the amplitude of the photoacoustic signal in the absorption peaks. However, this relationship is different for each isotope, which makes it difficult to extract the information of the isotopic ratio  $\delta^{13}\text{C}$ .

To extract this information, a theoretical model of the QEPAS signal is being developed in order to reproduce the signal obtained in the spectral swept range of the sensor [2][3]. The model output depends on the environmental characteristics of the air sample (CO<sub>2</sub> concentration, temperature and pressure) and on the operating characteristics of the sensor's QCL (variation of the emission power with the sweep, wavelength modulation index and residual amplitude modulation). It is expected that the adjustment of this model will allow the determination of the total CO<sub>2</sub> concentration and its isotopic composition more accurately.

The calibration is also being carried out using a reference instrument in atmospheric monitoring networks [2] (Picarro G2301). The figure below shows a picture of the system and a set of data obtained during a full day operation of the instrument.

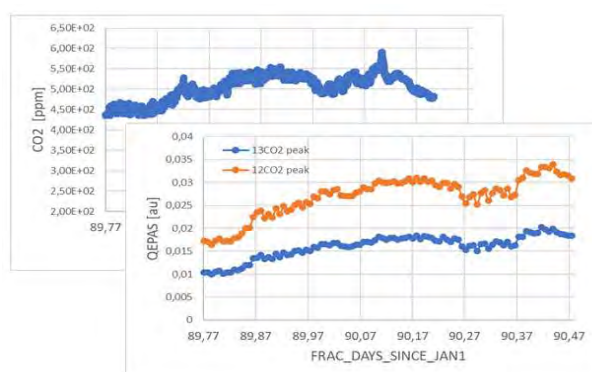


Fig. 1 QEPAS CO<sub>2</sub> analyser prototype and first results at demo site

## References

- [1] A. Sampaolo et al. "Quartz-enhanced photoacoustic spectroscopy for multi-gas detection: A review", *Analytica Chimica Acta*, Volume 1202, 338894 (2022). DOI: 10.1016/j.aca.2021.338894
  - [2] WMO: Expert group recommendations, 18th WMO/IAEA Meeting on Carbon Dioxide, Other Greenhouse Gases and Related Tracers Measurement Techniques (GGMT-2015), World Meteorological Organization (2016)
  - [3] Stéphane Schilt, Luc Thévenaz, "Wavelength modulation photoacoustic spectroscopy: Theoretical description and experimental results", *Infrared Physics & Technology*, Volume 48, Issue 2, 2006, Pages 154-162, ISSN 1350-4495, DOI: 10.1016/j.infrared.2005.09.001.
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# Quartz enhanced photoacoustic gas cell with optical multi-pass for detection of broad-spectrum gas molecules

Maxime Duquesnoy<sup>1</sup>, Jean-Michel Melkonian<sup>1</sup>, Raphaël Levy<sup>2</sup>, Guillaume Aoust<sup>2</sup>, Maxime Guais<sup>2</sup>,  
Grégory Maisons<sup>2</sup>, Léon Tran<sup>1</sup> and Myriam Raybaut<sup>1</sup>

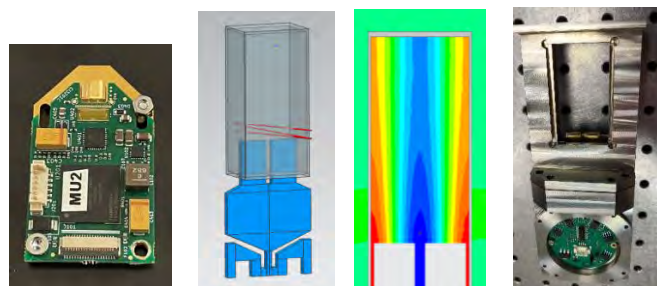
1. DPHY, ONERA, Université Paris-Saclay, 91123 Palaiseau, France

2. Mirsense, 1 Rue Jean Rostand, 91400 Orsay

**Short abstract:** We present the development of a photoacoustic gas detector composed of several longwave infrared QCLs and a QEPAS sensor for detection of chemical warfare agents at very low concentrations. The resonator and the lasers were arranged so as to maximize the SNR while minimizing the cell windows acoustic background.

Infrared laser absorption spectrometry is an established method for fast, selective, and non-intrusive measurement of trace level concentration of gaseous molecules in the atmosphere. Nevertheless, its application to heavy molecules is very challenging due to their very broad infrared spectrum, lacking the distinctive rovibrational lines of light molecules that can be easily separated from the absorption background and the instrumental baseline. To do so, one has to use either a laser with a very large spectral tunability (such as an extended-cavity quantum cascade laser [1]) or combine the outputs of several laser emitters, and the problem scales almost linearly with the number of target molecules [2]. For photoacoustic spectroscopy, detection of such large molecule spectra also requires to modulate the lasers in amplitude, instead of wavelength modulation, which creates an acoustic background often larger than the absorption signal itself.

To deal with these issues we have developed a photoacoustic gas sensor with a custom quartz tuning fork (QTF) and several quantum cascade lasers (QCL) units. The QTF is optimized for vibration at  $\sim 17$  kHz inside an acoustic resonant cavity, without the need to pass the laser between its prongs, a principle we already presented [3]. The signal is amplified and digitized with close proximity electronics separated from the gas chamber. The optical path was calculated with entrance and exit points located at pressure nodes, and the total length was the result of a compromise between the optical absorption and acoustic confinement. Three laser modules, each containing several DFB QCLs sharing the same gain region, were manufactured to sequentially emit a total of 32 wavelengths, chosen as to cover the absorption spectra of the main known chemical warfare agents in the  $1000\text{--}1250\text{ cm}^{-1}$  region. Within each module the beams are collimated with an array of flat InP microlenses and a small hemispherical ZnSe lens. Each laser emits around 1 mW and is operated in quasi-continuous-wave mode, with amplitude modulation at 17 kHz. A FPGA firmware was developed to synchronize laser operation and modulation with QTF signal demodulation.



**Fig. 1.** From left to right: laser module containing an array of  $\sim 15$  DFB QCLs; CAD view of the multipass acoustic cell; FEM simulation of the acoustic mode inside the cell; manufactured cell with the custom quartz tuning fork and its ADC electronics (windows have been removed).

We are currently validating the photo-acoustic cell against the initial finite element modelling and finalizing integration of the FPGA platform.

**Acknowledgements:** This research was funded by AID (Defence Innovation Agency) through the Rapid program (PARIS project no. 192906118).

## References

- [1] Stefano Zampolli et al., "A MEMS-Enabled Deployable Trace Chemical Sensor Based on Fast Gas-Chromatography and Quartz Enhanced Photoacoustic Spectroscopy," *Sensors*, vol. 20, p. 120, December 2019.
- [2] Chandra Kumar Naranbhai Patel, "Laser photoacoustic spectroscopy helps fight terrorism: High sensitivity detection of chemical Warfare Agent and explosives," *The European Physical Journal - Special Topics*, vol. 153, no. 1, pp. 1–18, 2008.
- [3] Maxime Duquesnoy et al., "Recent developments on QEPAS sensor using a radial resonator for mid-infrared measurements," in *CPASS*, Castellana Marina, 2023.



# Characterisation of a Multi-Pass Circular cell Using Photoacoustic Spectroscopy.

Oscar Bonilla-Manrique<sup>1</sup>, Alejandro Perez<sup>1</sup>, Sergio Jimenez<sup>1</sup>

*1. Universidad Carlos III de Madrid, Leganés, Madrid, 28911, Spain.*

**Short abstract:** In this document, the characterization of a circular Multipath Cell is presented using Photoacoustic Spectroscopy and three radially arranged capacitive microphones. These allowed the identification of three resonant modes ( $\sim 4000$ ,  $6800$  and  $8000$  Hz), and were validated by  $\text{NH}_3$  detection.

Optoacoustic spectroscopy (PAS) is a technique that utilizes the generation of acoustic waves in response to the absorption of light energy by a specimen. The absorption of light by a material leads to a local increase in temperature, which subsequently generates alterations in pressure within the surrounding environment. In this technique, the cell plays a pivotal role as a fundamental element, functioning as a cavity system that amplifies the acoustic signal generated by the absorption of light in the sample. This amplification capability enhances detection sensitivity and reduces noise levels, contributing to the overall performance of the optoacoustic spectroscopy system. This work proposes the characterization of a multi-pass cell (MPC), which will be validated in an optoacoustic spectroscopy architecture for the detection of dangerous gaseous substances, such as ammonia ( $\text{NH}_3$ ). By synchronizing the modulation frequency of the incident light with the resonance frequency of the cell, the efficiency of the photothermal signal detection is enhanced [1]. MPC-PAS systems offer distinct advantages due to the prolonged interaction time of the beam with the sample, thereby augmenting the optical path and enhancing the sensitivity to minute variations in the sample. Additionally, these systems offer enhanced sensitivity at low concentrations and improved selectivity. The multi-pass cell used is a circular cavity with a diameter of 10 cm, made up of numerous parabolic mirrors that facilitate multiple reflections of the optical beam inside the cell [2]. This configuration enables adaptable path lengths, straightforward alignment, and flexibility with respect to the detection technique. While these devices are typically employed for direct absorption spectroscopy, this document proposes their use as a circular resonator in a photoacoustic configuration. To this end, three capacitive microphones (FG-23329-P18, -53 dB, BW=10 kHz, KNOWLES ELECTRONICS) were installed inside the cell, equidistant from each other (1 cm) starting from the center of the cell, as shown in Fig 1a. Subsequently, the laser was focused inside the cell and modulated by a chopper. The modulation frequency of which was varied in a range from 1.5 kHz to 9 kHz with a step of 20 Hz. As illustrated in Fig. 1b, three primary resonant modes can be discerned for the three microphones, at approximate frequencies of 4000 Hz, 6800 Hz, and 8000 Hz.

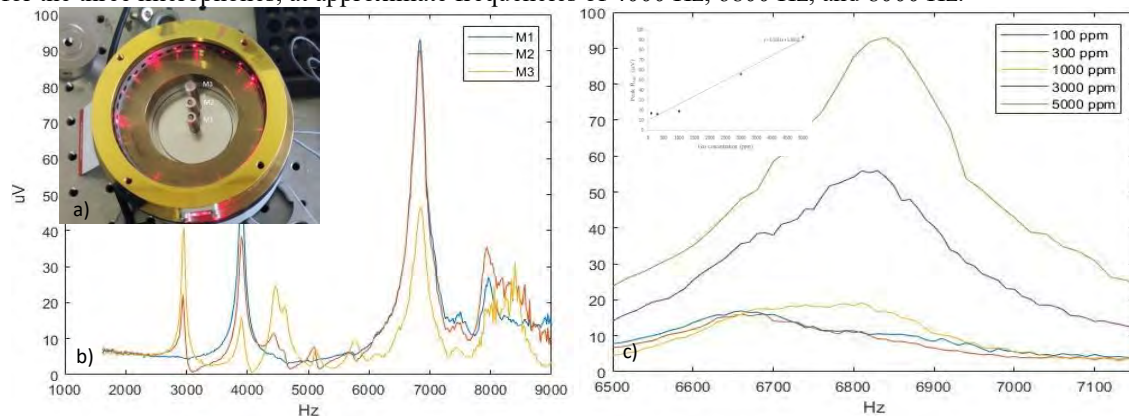


Fig 1. a) MPC with the 3 microphones. b) Resonance modes. c) Absorption at different concentrations.

To validate the complete system, different concentrations of  $\text{NH}_3$  were generated from 100 ppm to 5000 ppm by means of a gas mixer. The laser was configured to emit at a wavelength of 1532.2 nm, which coincides with an absorption line of  $\text{NH}_3$ , and sweeps were made around the most predominant resonance mode (6500–7150 Hz) to detect the acoustic signal in sensor M1. The ensuing results are presented in Fig. 1c, which showcases the graphs obtained at varying concentrations. The linearity of the measurement was evaluated according to the coefficient of determination ( $R^2$ ), yielding an  $R^2=0.91$ , thereby substantiating the high linearity of the system. Finally, the limit of detection (LOD) was 8 ppm, and was determined by evaluating the signal-to-noise ratio (SNR) at 1 and incorporating a standard deviation of the background noise.

[1] O. E. Bonilla-Manrique, P. Martín-Mateos, P. Acedo, and M. Ruiz-Llata, “Comparison of photoacoustic and wavelength modulation spectroscopy in a 3d-printed resonant gas cell,” vol. 12, p1-3 (2017).

[2] M. Graf, L. Emmenegger, and B. Tuzson, “Compact, circular, and optically stable multipass cell for mobile laser absorption spectroscopy,” Opt Lett, vol. 43, no. 11, p. 2434 (2018).



# Integrated Silicon Photonics



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# Subwavelength engineering of silicon photonics for nonlinear applications in the near-IR and mid-IR

Sara Toxqui-Rofriguez<sup>1</sup>, P. Nuño Ruano<sup>1</sup>, D. González-Andrade<sup>1</sup>, X. Le Roux<sup>1</sup>, D. Medina-Quiroz<sup>1</sup>, S. Edmond<sup>1</sup>, D. Marris-Morini<sup>1</sup>, E. Cassan<sup>1</sup>, L. Vivien<sup>1</sup>, and C. Alonso-Ramos<sup>1</sup>

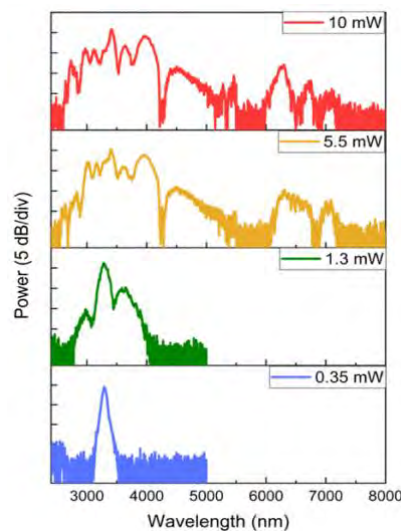
<sup>1</sup>Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, 91120 Palaiseau, France

**Short abstract:** Periodically patterning silicon with a subwavelength pitch opens new degrees of freedom to control light propagation in silicon photonic circuits with unprecedented flexibility. Here we present our most recent results on the use of subwavelength engineering for applications in nonlinear light generation in the near-IR and mid-IR.

The strong Kerr coefficient of silicon makes it a promising candidate for on-chip nonlinear generation of new optical frequencies, with a plethora of applications in fundamental and applied physics.

In the near-infrared (near-IR), Kerr nonlinearities are exploited for the implementation of photon-pair sources capable of generating multi-spectral entangled photon-pairs [1]. However, the substantially higher pump intensity and narrow wavelength separation between the photon-pairs and the optical pump impose stringent requirements that lie well-beyond capabilities of state-of-the-art silicon spectral filters. In this invited talk we will present an overview of our recent advances in the field of waveguide Bragg gratings for photonic noise reduction in silicon photon-pair sources, including the demonstration of a silicon photon-pair source with integrated pump-rejection filter achieving high visibility [2].

On the other hand, the wide transparency range of silicon (1.1-8  $\mu\text{m}$  wavelength) and the negligible two-photon absorption for wavelengths above 2  $\mu\text{m}$ , make this technology a very promising candidate for supercontinuum generation in the mid-IR. However, the use of the silicon-on-insulator technology in the mid-IR is limited by the absorption of the silica cladding for wavelengths above 3.5  $\mu\text{m}$ . Suspended silicon waveguides with metamaterial grating cladding allow overcoming the silica absorption limitation [3], while providing additional degrees of freedom in controlling waveguide dispersion. Here we will present our most recent results on the use suspended silicon waveguides for supercontinuum generation in the near-IR and mid-IR. As an example, Fig. 1 shows measured supercontinuum generation in a suspended silicon rib waveguide, expanding between 2.5  $\mu\text{m}$  and 7  $\mu\text{m}$  wavelength.



**Fig. 1** Experimental characterization of supercontinuum generation in suspended silicon rib waveguide.

## References

- [1] S. Azzini, D. Grassani, M. J. Strain, M. Sorel, L. G. Helt, J. E. Sipe, M. Liscidini, M. Galli, and D. Bajoni, “Ultra-low power generation of twin photons in a compact silicon ring resonator,” *Opt. Express*, **20**, 23100 (2010).
- [2] D. Oser, S. Tanzilli, F. Mazeas, C. Alonso-Ramos, X. Le Roux, G. Sauder, X. Hua, O. Alibart, L. Vivien, E. Cassan, and L. Labonté, “High-quality photonic entanglement out of a stand-alone silicon chip,” *Npj Quantum Inf.* **6**, 31 (2020).
- [3] J. Soler Penadés, A. Sánchez-Postigo, M. Nedeljkovic, A. Ortega-Moñux, J. G. Wangüemert-Pérez, Y. Xu, R. Halir, Z. Qu, A. Z. Khokhar, A. Osman, W. Cao, C. G. Littlejohns, P. Cheben, I. Molina-Fernández, and G. Z. Mashanovich, “Suspended silicon waveguides for long-wave infrared wavelengths,” *Opt. Lett.* **43**, 795 (2018).



# Graded index Silicon-Germanium photonics circuits for the mid-infrared spectral range

Delphine Marris-Morini<sup>1</sup>, Annabelle Bricout<sup>1</sup>, Javier Huertas Pedroche<sup>1</sup>, Victor Turpaud<sup>1</sup>, Hamza Dely<sup>1</sup>, Nooman El Bouchikhi<sup>1</sup>, Samson Edmond<sup>1</sup>, Carlos Alonso-Ramos<sup>1</sup>, Laurent Vivien<sup>1</sup>, Stefano Calcaterra<sup>2</sup>, Davide Impelluso<sup>2</sup>, Afonso De Cerdeira Oliveira<sup>2</sup>, Jacopo Frigerio<sup>2</sup>, Giovanni Isella<sup>2</sup>, Luca Lucia<sup>1</sup>, Gia Long Ngo<sup>1</sup>, Adel Bousseksou<sup>1</sup>, Raffaele Colombelli<sup>1</sup>, Victor Merupo<sup>3</sup>, Emilien Peytavit<sup>3</sup>, Jean-François Lampin<sup>3</sup>, Stefano Barbieri<sup>3</sup>, Philipp Täschler<sup>4</sup>, Mathieu Bertrand<sup>4</sup>, Barbara Schneider<sup>4</sup>, Jérôme Faist<sup>4</sup>

*1 Centre de Nanosciences et de Nanotechnologies, Université Paris-Saclay, CNRS, 91120, Palaiseau, France*

*2 L-Ness, Dipartimento di Fisica, Politecnico di Milano, Polo di Como, Via Anzani 42, 22100, Como, Italy*

*3-Institute of Electronics, Microelectronics and Nanotechnology, CNRS, Univ. Lille, France*

*4 Institute for Quantum Electronics, ETH Zurich, 8093 Zürich, Switzerland*

**Short abstract:** Recent developments of mid-infrared photonic circuits based on graded index Silicon-germanium waveguides will be presented. The presentation will focus on the demonstration of on-chip temporal compression of a QCL frequency comb source, demonstrating the generation of 1.75 ps pulses at 8  $\mu\text{m}$  wavelength, and on the demonstration of high speed integrated modulator, with an electro-optical bandwidth larger than 7 GHz.

Graded index Silicon-germanium waveguides present strong advantages for the development of mid-IR photonic circuits. They benefit from mature silicon (Si) fabrication processes while offering operation in an extended spectral range due to the wide transparency window of germanium (Ge) extending up to 15  $\mu\text{m}$ . Furthermore, by fine-tuning the Ge content in the SiGe alloy, it enables precise control of its optical properties (confinement and dispersion). In this context recent development will be presented.

## **1- On chip pulse compression :**

The generation of ultra short pulsed laser sources in the mid-IR using compact laser sources is of a prime interest for many applications related to absorption spectroscopy. It was shown previously that Fabry-Perot QCLs frequency comb operating around 8  $\mu\text{m}$  wavelength exhibit a linear chirp, which can be exploited to achieve temporal pulses from the quasi continuous output of the laser [1]. In this presentation, it will be shown that it is possible to achieve pulse compression on chip, using chirped Bragg grating filters integrated in graded index SiGe photonic circuits. The photonic circuit has been coupled with a QCL frequency comb and 1.75 ps pulses have been obtained.

## **2- High speed modulation :**

In mid-IR spectral range, high speed modulation can be obtained in SiGe by exploiting free carrier plasma dispersion effect. By embedding a Schottky diode embedded within the waveguide, it has been demonstrated previously that such an integrated modulator operates in a wide spectral range from 5 to 9  $\mu\text{m}$  wavelength [2]. However in the previous demonstration, the high speed characterization was limited by the electro-optical bandwidth of the commercially available detector used in the set-up. It will be shown that recent experiments have been conducted using a high speed Quantum well infrared photodetector (QWIP) [3]. Interestingly, it is now possible to conclude that the modulator reaches an electro-optical bandwidth higher than 7 GHz.

In conclusion, recent developments show that graded index SiGe photonics circuits is a mature platform where advanced optical functions can be implemented for light manipulation on chip. By proper coupling with efficient laser sources and photodetectors, these results pave the way to a plethora of demonstrations related with absorption spectroscopy and sensing.

**Acknowledgement:** This project has received funding from the European Union's Horizon Europe research and innovation programme (101128598 - UNISON) and from the European Research Council (ELECTROPHOT - 101097569)

## **References**

- [1] P. Täschler, et al, Femtosecond pulses from a mid-infrared quantum cascade laser. *Nat. Photon.* **15**, 919–924 (2021).
- [2] T.H.N. Nguyen, et al, 1 GHz electro-optical silicon-germanium modulator in the 5-9  $\mu\text{m}$  wavelength range, *Optics Express*, **30**, (26), 47093 (2022).
- [3] Q. Lin et al. , Real-time, chirped-pulse heterodyne detection at room temperature with 100 GHz 3-dB-bandwidth mid-infrared quantum-well photodetectors, *Optica* **10**, 1700, (2023)

# Silicon Photonics for Mid-IR Sensing

Goran Z. Mashanovich<sup>1</sup>, Siyu Chen<sup>1</sup>, James Fernando<sup>1</sup>, Aneesh V. Veluthandath<sup>1</sup>, Dolnapa Yamano<sup>2</sup>, Sam Thompson<sup>2</sup>, Samuel McQuillan<sup>1</sup>, Rand Ismaeel<sup>1,3</sup>, Panagiotis Galanis<sup>3</sup>, Jon Heffernan<sup>4</sup>, Kristian M. Groom<sup>4</sup>, Longqi Zhou<sup>4</sup>, Tianhui Hu<sup>1</sup>, Matthew C. Mowlem<sup>1</sup>, Pin Dong<sup>5</sup>, Yue Wang<sup>5</sup>, Thomas F. Krauss<sup>5</sup>, David J. Rowe<sup>1</sup>, Colin J. Mitchell<sup>1</sup>, Ganapathy S. Murugan<sup>1</sup>, Milos Nedeljkovic<sup>1</sup>

1. Optoelectronics Research Centre, University of Southampton, Southampton, SO17 1BJ, UK

2. School of Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton, Southampton, SO17 1BJ, UK

3. National Oceanography Centre, Southampton, SO14 3ZH, UK

4. Department of Electronic and Electrical Engineering, University of Sheffield, Sheffield, S10 2TN, UK

5. School of Physics, Engineering and Technology, University of York, Heslington, York YO10 5DD, UK

**Short abstract:** We report on the development of mid-infrared silicon photonics sensors for healthcare and environmental monitoring. We show the realisation of germanium-on-silicon absorption spectroscopy sensors for therapeutic drug monitoring and cancer detection, as well as silicon-on-insulator gas sensors. We also report integration of mid-IR sources and detectors with mid-IR silicon photonic circuits.

Monitoring therapeutic drug levels in bodily fluids is a vital component of clinical care. Traditionally, this process, known as therapeutic drug monitoring (TDM), relies on techniques such as liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). While effective, these methods are restricted to centralised laboratories and cannot deliver the rapid feedback often needed by healthcare providers. In our work, we demonstrate that Ge-on-Si waveguides can serve as an alternative platform for drug detection. A key obstacle in this context is the significant mid-infrared absorption caused by naturally occurring substances in serum. To overcome this, we developed a strategy to eliminate the interfering signals from lipids, proteins, and water-soluble molecules present in the sample. Using phenytoin, a common antiepileptic medication, as a case study, we were able to accurately measure drug concentrations at clinically significant levels (10 µg/mL), offering a promising and efficient solution for real-time TDM [1]. We have also conducted a lung cancer detection study and have obtained promising results [2].

Whether to incorporate a light source or a detector directly onto a transducer chip depends largely on the specific application. In medical diagnostics, for instance, sensors are typically not reused due to contamination concerns, making the transducer component single-use. In such cases, integrating a laser source on-chip would not only be economically impractical but also environmentally unsustainable. On the other hand, integrating a detector tends to be more feasible, both in terms of cost and technical complexity. A practical solution may involve co-integrating the transducer and detector, minimising alignment challenges by limiting them to just one optical interface, namely between the external source and the chip. In contrast, for applications like atmospheric gas sensing where disposability is not required, fully integrated systems offer clear advantages, including a smaller device footprint and better resilience to mechanical vibrations [3].

We report on gas detection using silicon waveguides functionalised with cryptophane-enriched membranes. Additionally, we introduce an innovative approach for the hybrid integration of quantum cascade laser (QCL) bars with Ge-on-Si waveguides. The QCL bars are mounted via flip-chip bonding onto a Ge-on-Si substrate without the need for active alignment, achieving end-fire coupling efficiencies as high as 45% (equivalent to a 3.5 dB insertion loss) during pulsed mode operation. Optical measurements suggest that between 20 and 30 mW of power is delivered into the waveguide. This passive assembly technique, paired with a CMOS-compatible photonic integration platform, provides a scalable route toward compact and fully integrated mid-IR photonic solutions for sensing applications.

## References

- [1] P. Dong, K. Li, D. J. Rowe, T. F. Krauss, and Y. Wang, "Protocol for Therapeutic Drug Monitoring Within the Clinical Range Using Mid-infrared Spectroscopy," *Anal. Chem.* **96**, 19021 (2024).
- [2] D. J. Rowe, S. L. Hill, V. M. Goss, A. Hicks, P. A. J. Crosbie, M. E. J. Callister, P. W. M. Johnson, and G. Z. Mashanovich, "Lung Cancer Detection in a High-risk Screening Cohort Using Machine Learning-assisted ATR-FTIR Spectroscopy of Serum," *Photonics West 2025*, San Francisco, USA, 25-30 January 2025.
- [3] C. J. Mitchell, T. Hu, S. Sun, C. J. Stirling, M. Nedeljkovic, A. C. Peacock, G. T. Reed, G. Z. Mashanovich, and D. J. Rowe, "Mid-Infrared Silicon Photonics: from Benchtop to Real-world Applications," *APL Photonics* **9**, 080901 (2024).
- [4] G. Z. Mashanovich, C. J. Mitchell, C. Wei, S. McQuillan, R. Ismaeel, J. Heffernan, K. M. Groom, T. Hu, D. Yamano, S. Thompson, D. Miall, M. C. Mowlem, D. J. Rowe, and M. Nedeljkovic, "Silicon Photonics for the Mid-IR," *Photonics West 2025*, San Francisco, CA, USA, 25 – 30 January 2025.



# On-Chip Waveguide Sensor Module for Precision MIR Spectroscopy

Ragnar Seton, Jehona Salaj, Roman Zakoldaev, Marek Vlk, Jan Viljanen, and Jana Jágerská

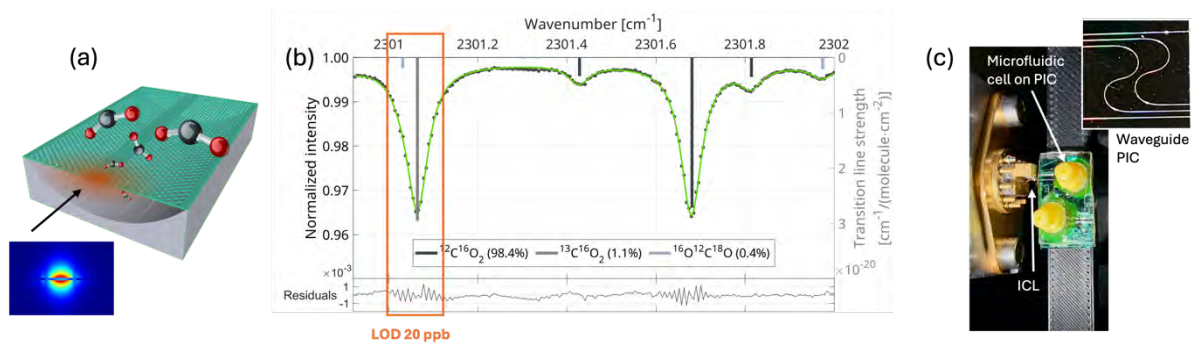
Department of Physics and Technology, UiT The Arctic University of Norway, Tromsø, Norway

**Short abstract:** We report on a chip-scale, waveguide-based sensor module integrated with an interband cascade laser and a microfluidic cell. Combined with direct laser absorption spectroscopy, this module achieves sub-ppm detection of  $^{13}\text{CO}_2$  and demonstrates the capability for precise  $\delta^{13}\text{C}$  isotope ratio measurements.

Over the past few decades, the development of portable, high-precision trace gas sensors utilizing infrared (IR) spectroscopy has made significant strides. However, the traditional implementation of gas cells using bulk optics has maintained a large instrument size and sample volume. Optical waveguides, processed lithographically on a photonic chip, have emerged as a promising solution for instrument integration. Yet, conventional dielectric waveguides have encountered challenges such as substantial spectral noise and high propagation losses, which limit detection sensitivity to tens or hundreds of parts per million (ppm).

The Photonic Sensors Group at UiT The Arctic University of Norway in Tromsø focuses on developing specialized mid-infrared waveguides for IR laser absorption spectroscopy. By introducing air-like modes, we have enhanced light-matter interaction with surrounding gases, reduced propagation losses, and suppressed reflection-induced spectral noise to below detectable levels [1]. Our latest design features a thin-film free-standing waveguide with microstructured cladding, enabling  $\text{CO}_2$  detection down to 20 parts per billion (ppb) and achieving the first on-chip detection of  $\delta^{13}\text{C}$  in  $\text{CO}_2$  with precision of 0.2‰. This breakthrough has elevated on-chip detection sensitivities to levels comparable with high-end, bulky instruments, Fig. 1(a, b) [2].

In this contribution, we report on the performance of a new miniature module that incorporates the aforementioned sensor. This module integrates the sensor with a microfluidic cell of 20 microliters sensing volume and utilizes an interband cascade laser (ICL) that directly butt-couples light into the waveguide without any free-space optics, Fig. 1(c). We demonstrate that even in this compact form, spectral tuning remains unaffected, and the sensor performance is comparable to that of a laboratory setup. This development represents a significant step towards full sensor integration and the realization of the most compact precision sensor for environmental, space, and biotechnology applications.



**Fig. 1** (a) Schematic of the free-standing waveguide design with simulated field distribution. (b) Example spectrum showing two  $\text{CO}_2$  isotope absorption lines obtained using a free-space laboratory setup. (c) Photograph of a sensor chip equipped with a microfluidic cell, butt-coupled to an interband cascade laser.

## References

- [1] M. Vlk, A. Datta, S. Alberti, H. D. Yallev, V. Mittal, G. S. Murugan, J. Jágerská, "Extraordinary evanescent field confinement waveguide sensor for mid-infrared trace gas spectroscopy," *Light Sci. Appl.*, **10**, 26 (2021)
- [2] J. Salaj, M. Vlk, R. Zakoldaev, R. Seton, J. Čtyroký, S. Alberti, A. Aksnes, J. Jágerská, "Suspended nanophotonic waveguide for isotope-specific  $\text{CO}_2$  detection," *Optica* **11**, 1654-1662 (2024)

# Suspended Waveguide Enhanced Raman Spectroscopy for Trace Molecule Sensing

Jan Viljanen<sup>1</sup>, Martin Feiler<sup>1</sup> and Jana Jägerská<sup>1</sup>

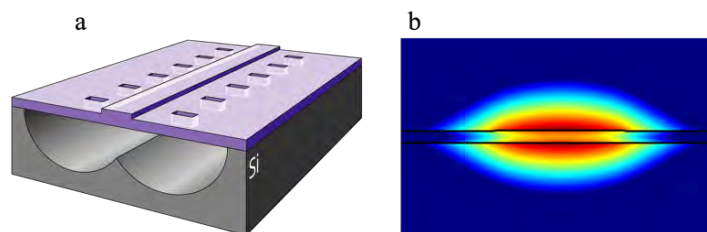
*1. Department of Physics and Technology, UiT The Arctic University of Norway, Tromsø, Norway*

**Short abstract:** Nanophotonic waveguides are a key solution for the miniaturization of Raman sensors without compromising sensitivity and selectivity. Suspended rib waveguide design with robust fabrication process is projected to substantially outperform both confocal Raman and previous waveguide designs. It will be used for trace molecule sensing with full on-chip integration potential.

Raman spectroscopy is a powerful and versatile analytical technique widely used in both analytical chemistry and environmental sciences due to its ability to provide detailed molecular information without the need for extensive sample preparation. However, due to the inherently weak nature of the Raman interaction, Raman applications require bulky and expensive devices to overcome the poor signal-to-pump-power ratio, i.e., the poor conversion efficiency. In traditional Raman applications, the conversion efficiency is limited by the low light-sample interaction volume and inefficiency of the signal collection.

Nanophotonic waveguides offer a promising solution to these challenges. They significantly increase the interaction volume along the waveguide length and enhance both Raman scattering and collection efficiency. With waveguide-enabled multi-centimeter interaction length, waveguide-enhanced Raman spectroscopy (WERS) is projected to outperform confocal Raman spectroscopy in sensitivity by more than 100 times. Additionally, nanophotonic waveguides are a key solution for the miniaturization of optical sensors, allowing for reduced size without compromising sensitivity and selectivity.

In this work, we present a nanophotonic suspended rib waveguide [1] (Fig. 1) as a highly promising solution for on-chip waveguide enhanced Raman spectroscopy (WERS). Operating at a wavelength of 780 nm in an air environment, the waveguide achieves a 103% TM mode evanescent field confinement factor leading to theoretical Raman conversion efficiency of 0.9. This is about 5 times higher than what is achievable with slot waveguides [2], previously highlighted as an optimal waveguide design for WERS. In addition, membrane waveguide design surmounts previously presented waveguides [3] due to the reduced Raman background from the waveguide material and easy and robust fabrication.



**Fig. 1** a) Schematic of the membrane waveguide design, b) fundamental TM mode with 103% evanescent field confinement factor and 0.9 Raman conversion efficiency in air.

The waveguide used in this work is based on 150 nm thick low-stress silicon nitride (SiN) platform that is grown on Silicon (Si) substrate. The ~5 nm high rib was produced with shallow ICP RIE etching followed by two-step etching process to i) provide openings alongside the waveguide down to the Si substrate and ii) to isotropically under-etch SiN to release the membrane structure. The waveguide design is feasible for chemical analysis both in gas and liquid phases. The next steps are to apply the sensor to trace molecule sensing in liquids and develop it towards an integrated device enabling comprehensive in-situ environmental sensing.

## References

- [1] M. Vlček, A. Datta, S. Alberti, H. D. Yalçın, V. Mittal, G. S. Murugan, & J. Jägerská, "Extraordinary evanescent field confinement waveguide sensor for mid-infrared trace gas spectroscopy," *Light: Science & Applications*, **10**, (2021)
- [2] A. Dhakal, A. Raza, F. Peyskens, A. Z. Subramanian, S. Clemmen, N. Le Thomas, & R. Baets, "Efficiency of evanescent excitation and collection of spontaneous Raman scattering near high index contrast channel waveguides," *Optics express*, **23**, (2015)
- [3] J. Zhao, X. Cao, W. Xu, & S. Xu, "Waveguide-based Raman enhancement strategies," *Journal of Raman Spectroscopy*, **55**, (2024)

# Industrial Applications



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# Hydrogen detection via Raman-based sensor

Fabio Melison<sup>1</sup>, Lorenzo Cocola<sup>1</sup> and Luca Poletto<sup>1</sup>

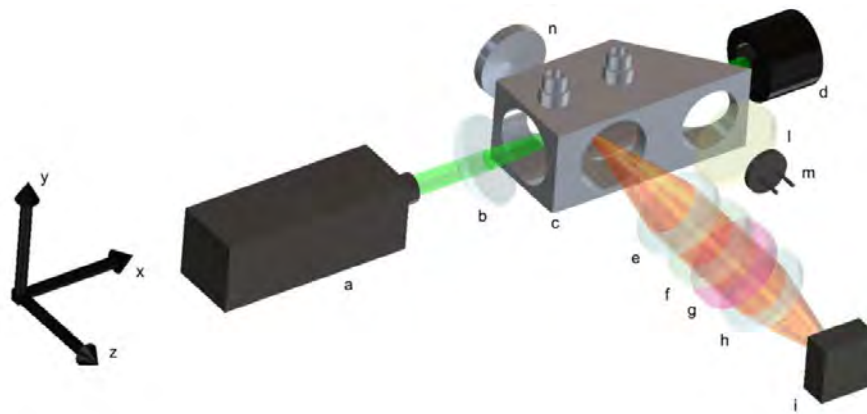
*1. CNR-IFN, National Research Council of Italy – Institute for Photonics and Nanotechnologies, Via Trasea 7, 35131 Padova, Italy*

**Short abstract:** A non-dispersive Raman spectroscopy system is presented suitable for the detection of hydrogen, nitrogen and oxygen. It utilizes band-pass filters for the selective detection of the Raman-emission. Compared to a dispersive setup, it achieves lower detection limits (40 ppm H<sub>2</sub> at 3 bars) with simplified design, fewer components, and improved performance across the operative ranges of sample pressures and camera integration times.

Hydrogen is increasingly being considered as renewable energy carrier. This interest is driven by its favorable properties: it is lightweight, storable, highly reactive, has a high energy content per unit mass, and can be produced on an industrial scale. Along the entire hydrogen supply chain, from production to transportation and end-use, it is critical to: (i) comply with relevant regulations, (ii) maximize the efficiency of energy conversion systems, (iii) ensure safety in all environments associated with hydrogen handling and transport. Several measurement techniques are utilized depending on the application-specific demands, including sensitivity, time response and recovery times, full-scale range, and cross-sensitivity to impurities.

Raman spectroscopy provides a non-intrusive way to analyze gaseous samples. It requires only a laser to pass through the gas and optical access for detecting the scattered light, making it ideal for in-situ monitoring. [1,2,3]. A Raman system designed for the detection of hydrogen, nitrogen, and oxygen is presented. The system utilizes a non-dispersive approach, wherein the Raman scattering signals of the three target molecules are selectively detected using different band-pass filters which allow the proper wavelengths to pass through the filters themselves and to be collected by the camera. The performance of this design is compared to a dispersive approach, which employs a diffraction grating spectrometer to analyze the spectrum. To evaluate system performance, a certified gas mixture (2% H<sub>2</sub>, 77.1% N<sub>2</sub>, 20.9% O<sub>2</sub>) was pressurized into a gas cell at 1–3 bar. Raman signals were recorded using both setups across integration times of 2–10 s. The Raman emission is triggered by a 532nm DPSS Nd:YAG laser source with an optical power of 1.5W. The advantages of the non-dispersive configuration include a simplified design, reduced use of optical and mechanical components, and easier assembly and alignment. The non-dispersive approach leads to lower LODs in a simpler and compact optical setup.

The H<sub>2</sub> LODs are 345 ppm and 980 ppm for the non-dispersive and dispersive approaches, respectively (1,5 bar sample pressure, 2 s integration). By increasing the sample pressure and camera integration time (3 bar and 10 s), the H<sub>2</sub> LOD for the non-dispersive approach decreases to 40 ppm.



**Fig. 1** System schematic. a) laser source. b) focusing lens. c) gas cell. d) beam dump. e,h) collecting lenses. f) long-pass filter. g) band-pass filter. i) camera. l) diffuser. m) photodiode. n) back-reflection mirror.

## References

- [1] Dal Moro R, Melison F, Cocola L, Poletto L. Raman Spectroscopy for Temporally Resolved Combustion Gas Diagnostics. *Applied Spectroscopy*. 2024;78(12):1263-1269. doi:10.1177/00037028241277575.
- [2] D.V. Petrov, I.I. Matrosov, M.A. Kostenko, Multipass Raman gas analyzer for monitoring of atmospheric air composition, *Optics & Laser Technology*, <https://doi.org/10.1016/j.optlastec.2022.108155>.
- [3] F. Melison et al "Natural gas and hydrogen-enriched natural gas composition measurements by industrial-grade Raman spectroscopy", *Proc. SPIE 13026*; <https://doi.org/10.1117/12.3012835>.

# **Real time monitoring of H<sub>2</sub>S emissions at the Pisciarelli fumarolic field (Campi Flegrei caldera) using a compact Quartz-Enhanced Photoacoustic sensor**

**Elefante, A.<sup>1,2</sup>, Olivieri M.<sup>1</sup>, Lombardi L.<sup>3</sup>, Spagnolo V.<sup>1,3</sup>, Spagnolo, D.<sup>1</sup>, Massaro S.<sup>4</sup>, Sulpizio R.<sup>5</sup>, Dellino P.<sup>5</sup>,  
Rufino F.<sup>6</sup>, Caliro S.<sup>6</sup>, Costa A.<sup>4</sup> and Patimisco P.<sup>1,3</sup>**

<sup>1</sup> PolySense Lab, Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari, 70126 Italy

<sup>2</sup> CNR, Istituto di Fotonica e Nanotecnologie, Sede di Bari, Italy

<sup>3</sup> PolySense Innovations srl, Via Amendola 173, Bari, 70126 Italy

<sup>4</sup> Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Bologna, 40126 Bologna, Italy

<sup>5</sup> Dipartimento Di Scienze Della Terra e Geoambientali, Università di Bari, Italy

<sup>6</sup> Istituto Nazionale di Geofisica e Vulcanologia, Osservatorio Vesuviano, Napoli, Italy

Monitoring the volcanic plume emissions of dormant volcanoes and restless calderas reveals essential information on the sub-surface magmatic and hydrothermal processes, providing an essential tool for improving the surveillance of active volcanoes, especially during the unrest phases. Together with the predominant emissions of water vapor (H<sub>2</sub>O) and carbon dioxide (CO<sub>2</sub>), monitoring the sulfur degassing, in terms of hydrogen sulphide (H<sub>2</sub>S) and sulfur dioxide (SO<sub>2</sub>), is a priority due to its significant atmospheric and climatic impacts. To achieve reliable and continuous monitoring under the challenging conditions typical of volcanic environments, compact and robust sensors are required, capable to guarantee high selectivity and sensitivity with detection limits in the part-per-million (ppm) range in the complex and variable volcanic plume. Moreover, a fast response time on the order of seconds is a precious asset for effectively tracking rapid changes in gas emissions. Quartz Enhanced Photoacoustic Spectroscopy (QEPAS) sensors fulfil these requirements by using a quartz tuning fork to detect sound waves generated by the interaction of the target gas with infrared modulated light. In addition, QEPAS sensors overcome the cross-interference and long recovery-time limitations, offering an advantageous alternative to conventional electrochemical sensors.

Here we report on the realization and implementation of a multi-gas sensor system composed of an electronic hygrometer for temperature and H<sub>2</sub>O monitoring, a commercially available CO<sub>2</sub> sensor and a compact QEPAS sensor for the detection of H<sub>2</sub>S in volcanoes environment. The QEPAS sensor employed a DFB diode laser targeting the H<sub>2</sub>S absorption line at 3792.90 cm<sup>-1</sup> and an acoustic module composed of a T-shaped quartz tuning fork coupled with micro-resonator tubes. The QEPAS sensor was optimized and calibrated in laboratory using a certified gas mixture of 250 ppm H<sub>2</sub>S in nitrogen, reaching a 1-σ minimum detection limit of 1.6 ppm with an integration time of 1 s, at a working pressure of 100 Torr. Field tests were carried out through continuous, real-time measurements at the Pisciarelli fumarolic field (Campi Flegrei caldera, southern Italy) with the system operating for several hours for three days. Measurements were taken at varying distance from the main fumarolic vent (from few to tens of meters), demonstrating the sensor capability to track rapid fluctuations of H<sub>2</sub>S concentrations within the plume. At the closest distance, H<sub>2</sub>S peaks of tens of ppm were detected and positive correlation with the CO<sub>2</sub> emission was retrieved. These results fully demonstrated the applicability of the multi-gas system for monitoring H<sub>2</sub>S concentrations and the CO<sub>2</sub>/H<sub>2</sub>S ratio in volcanic environments.



# Realization of an automatic waste material recognition system for waste recycling

Claudio Fratini<sup>1</sup>, Andrea De Iacovo<sup>1</sup>, Andrea Ballabio<sup>2</sup>, Jacopo Frigerio<sup>3</sup>, Giovanni Isella<sup>3</sup>, Andrea Ria<sup>4</sup>, Paolo Bruschi<sup>4</sup>, Lorenzo Colace<sup>1</sup>

1. Roma Tre University, Department of Industrial, Electronic, and Mechanical Engineering

2. EYE4NIR S.r.l.

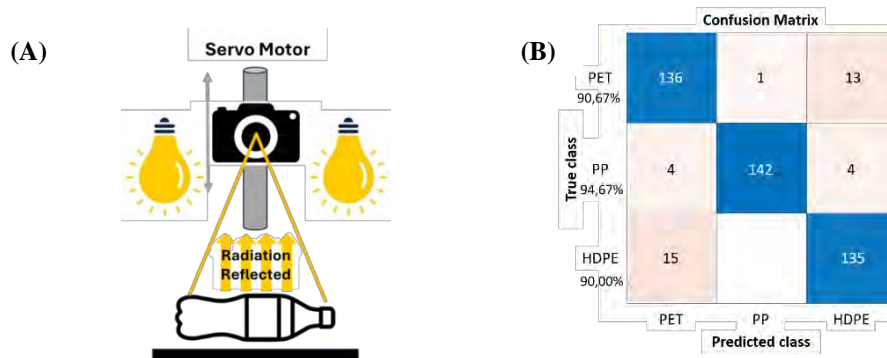
3. Politecnico di Milano, Department of Physics

4. University of Pisa, Department of Information Engineering

**Short abstract:** The research focuses on developing an automatic system to identify and sort disposable waste using a dual-band photodetector array operating in visible and near-infrared wavelengths. By combining spectral and spatial data through classification algorithms, the system is able to classify common waste material like PET, PE-HD and PP.

The research focuses on developing an automatic system for the identification of plastic waste materials, with the aim of correctly sorting and recycling them. The identification is based on the analysis of the reflectivity spectrum acquired through a one-dimensional array of 128 dual-band photodetectors similar to the one shown in [1]. The photodetectors selected for this study, patented by the company Eye4NIR s.r.l., are based on silicon-germanium technology and operate in both the visible and short-wave infrared spectrum. Their spectral response can be electronically tuned by varying the bias voltage. The linear photodetector array is placed in the image plane of a standard camera lens, focused onto the sample under analysis. Multiple acquisitions ( $n$ ) of the same spatial line were performed for each sample by varying the applied voltage each time. The result is an image of dimensions  $n \times 128$  combining both spatial and spectral information. This procedure is repeated  $m$  times for each sample by vertically translating the photodetector array using an external servo motor, acquiring in that way different spatial lines of the same object.

A simplified schematic of the setup is shown in Fig. 1A: radiation from two incandescent lamps is reflected by the samples and captured by the sensors. At first, we have focused on the study of samples made by major plastic categories such as PET, PE-HD, and PP. The resulting dataset was preprocessed to reduce the influence of outliers and was used to train various classification models in MATLAB. Their performance was evaluated using Cross-Validation techniques. The best result has been obtained with the Bagged Trees algorithm (91.77% global accuracy), whose confusion matrix is shown in Fig. 1B.



**Fig. 1:** (A) Simplified representation of the setup used for the acquisitions;  
(B) Confusion Matrix of the three plastic classes obtained by the Cross-Validation of the trained model (91.77% global accuracy).

Additional tests were conducted by introducing samples of other materials such as LDPE, paper, metal, and glass. As expected, the introduction of more classes reduced the classification accuracy. Several tests were performed on the trained model, including evaluation with a test dataset composed of different samples. Comparison with a similar previous research made with a single Eye4NIR's sensor and more uniform samples demonstrated increased accuracy due to the inclusion of spatial information in the model, thanks to the employment of the linear photodetector array [2].

## References

- [1] A. De Iacovo, F. Mitri, A. Ballabio, J. Frigerio, G. Isella, A. Ria, M. Cicalini, P. Bruschi, L. Colace, "Dual-Band Ge-on-Si Photodetector Array With Custom, Integrated Readout Electronics", *IEEE Sensors J.* **22**, 3172-3180 (2022)
- [2] A. Manakkakudy Kumaran, A. De Iacovo, A. Ballabio, J. Frigerio, G. Isella, L. Colace, "Waste Material Classification Based on a Wavelength-Sensitive Ge-on-Si Photodetector", *Sensors* **24**, 6970 (2024)

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# Spectroscopic study of Volatile Organic Compounds for the assessment of coffee authenticity

Marilena Giglio<sup>1</sup>, Arianna Elefante<sup>2</sup>, Lavinia Mongelli<sup>1</sup>, Adriana Bux<sup>1</sup>, Andrea Zifarelli<sup>1</sup>, Giansergio Menduni<sup>1</sup>, Pietro Patimisco<sup>1</sup>, Andrea Caratti<sup>3</sup>, Cecilia Cagliero<sup>3</sup>, Erica Liberto<sup>3</sup>, Chiara Cordero<sup>3</sup>, Luciano Navarini<sup>4</sup>, Vincenzo Spagnolo<sup>1</sup> and Angelo Sampaolo<sup>1</sup>

1. PolySenSe Lab, Physics Department, Polytechnic University and University of Bari, Via G. Amendola, 173, 70126, Bari

2. Consiglio Nazionale delle Ricerche (CNR), Istituto di Fotonica e Nanotecnologie, Sede di Bari, 70126, Bari, Italy

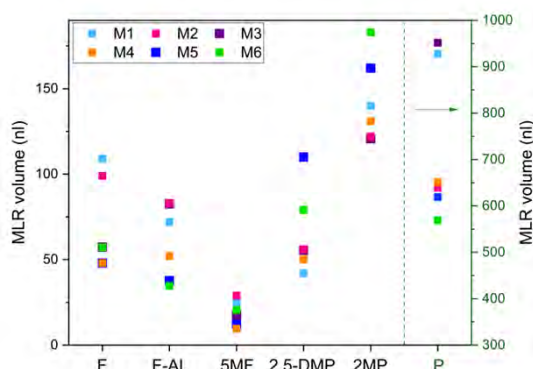
3. Dipartimento di Scienza e Tecnologia del Farmaco, Università di Torino, Via Pietro Giuria 9, 10125, Torino, Italy

4. Illycaffè S.p.A., via Flavia 110, 34147 Trieste, Italy

**Short abstract:** This study aimed at defining the infrared spectral signatures of six volatile organic compounds (VOCs) of relevant interest for coffee bean authentication and quality control using Fourier Transform Infrared Spectroscopy. The achieved results demonstrate the potentiality of coffee fingerprinting by VOC's signature in the absorption spectra for discriminating coffee origin.

Coffee authentication and quality control is addressing an increasing importance, being that coffee is among the main traded crops and one of the most consumed beverages worldwide. Many coffee studies rely on the analysis of its volatile chemical composition, which is intrinsically related to the sensed aroma. The coffee volatile organic compounds (VOCs) matrix is the result of several cascade processes determining the final sensorial profile. However, several factors, including species and cultivars of coffee and other parameters related to geographical origin, such as climate, soil, temperature, and altitude, lead to distinguishable final products [1].

In this work, Fourier Transform Infrared Spectroscopy (FTIR) was employed to acquire high-resolution IR spectra of a set of compounds simplifying the complexity of coffee volatiles. Six molecules have been selected in this study as fingerprinting set, based on both their abundance and discriminating power in coffee authentication and quality control. These molecules include Pyridine (P), 2-Methylpyrazine (2MP), 2,5-Dimethylpyrazine (2,5-DMP), Furfural (F), 5-Methylfurfural (5MF), and Furfuryl Alcohol (F-AL) [2]. Six coffee odorant mixtures simulating the volatile composition of coffee beans for the selected target analytes from different geographical origins have been analyzed to investigate the capability to discriminate the coffee origins by the analysis of the spectral features of the six selected VOCs. Differently from the standard FTIR analysis aiming at samples' classification or clustering, without a precise discrimination and quantification of single compound in the mixture, we applied multi-linear regression (MLR) in both cases to estimate the absolute content of each molecule starting from single-molecule reference. The obtained results are shown, for each mixture, in Fig. 1.



**Fig. 1** Trends of variation in each VOCs in the six mixtures, based on the volumes retrieved by the FTIR spectra analysis. The green dotted line and arrow indicate the volume scale used for Pyridine, shown on the right of the graph.

## References

- [1] P.R.A.B. Toledo, L. Pezza, H.R. Pezza, and A.T. Toci, "Relationship Between the Different Aspects Related to Coffee Quality and Their Volatile Compounds," *Compr. Rev. Food Sci. Food Saf.*, **15**, 705–719 (2016)
- [2] L. Mondello, R. Costa, P.Q. Tranchida, P. Dugo, M. Lo Presti, S. Festa, A. Fazio, and G. Dugo, "Reliable characterization of coffee bean aroma profiles by automated headspace solid phase microextraction-gas chromatography-mass spectrometry with the support of a dual-filter mass spectra library," *J. Sep. Sci.*, **28**, 1101–1109 (2005)

# Time-resolved gas detection using mid-infrared upconversion spectroscopy

Yueyu Lin<sup>1</sup>, Roderik Krebbers<sup>1</sup>, Paola Formica<sup>1,2</sup>, Amir Khodabakhsh<sup>1,3</sup>, and Simona M. Cristescu<sup>1</sup>

1. Life Science Trace Detection Laboratory, IMM, Radboud University, 6525 AJ Nijmegen, The Netherlands

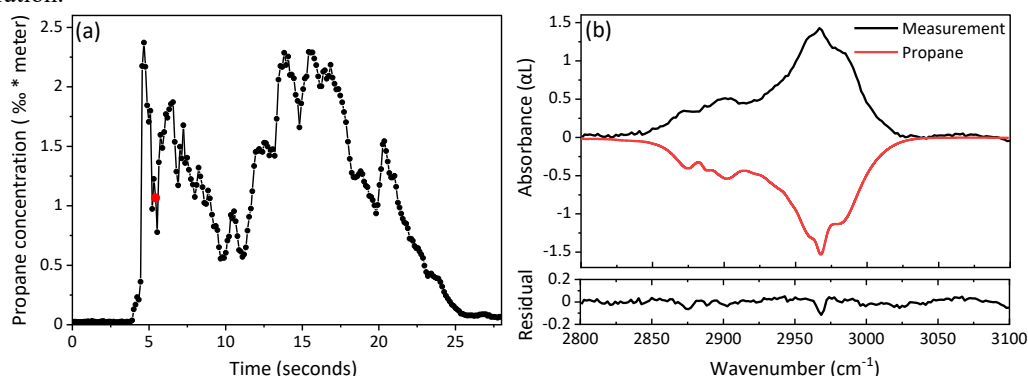
2. Department of Physics, University of Bari, Via G. Amendola 173, Bari 70125, Italy

3. Circular Chemical Engineering, Faculty of Science and Engineering, Maastricht University, 6229 GS Maastricht, The Netherlands

**Short abstract:** We report a mid-infrared upconversion-based spectroscopic system achieving a time resolution up to 27 ms and evaluate its performance in real-time leak detection in open-path spectroscopy and tracking evaporation processes in open-cell setups.

Fast and sensitive detection in broadband mid-infrared (MIR) spectroscopy has long posed significant challenges. The developments in high brightness and spatially coherent fiber-based MIR supercontinuum (SC) sources enabled sensitive, broadband absorption spectroscopic measurements by providing intense output light across a broad spectrum. However, the acquisition rate of the broadband absorption spectra is usually restricted by the required mechanical movement inside the spectrometer. For example, Fourier-transform infrared spectroscopy (FTIR) requires the movement of a scanning arm and usually provides a time resolution between 0.4 – 2 s [1], while grating-based spectroscopy with a rotating grating can provide a time resolution of 0.1 s [2]. Alternatively, upconversion spectroscopy can be used to convert the MIR light into near-infrared (NIR). Photodetector arrays (e.g., CCD) can capture the entire NIR spectrum simultaneously, significantly improving the measurement speed. Thus, a grating-based upconversion spectrometer can provide both a high detection sensitivity and temporal resolution as the CCD removes the need for mechanically moving parts [3].

Here, we present a time-resolved detection system using a MIR SC source ( $\sim 1.8 - 4.2 \mu\text{m}$ , SuperK MIR, NKT Photonics) and a grating-based upconversion spectrometer ( $\sim 2.8 - 4.2 \mu\text{m}$ , S3055, LNIR). We evaluated the system's performance in two applications: leak detection in an open-path configuration and evaporation tracking in an open-cell setup. In both applications, the laser beam is sent through ambient air for direct interaction with the gas. However, open-path experiments use retroreflectors to reflect the laser beam over distances of tens to hundreds of meters, while open-cell setups employ a cavity of tens of centimeters with two concave mirrors to achieve multipass detection. For the open-path configuration, we conducted an outdoor, controlled propane release experiment. The distance between the system and the retroreflectors was 76.5 m, achieving a total 153-meter pathlength. The release point was set under the laser beam at 38 meters from the system. A propane detection limit of  $\sim 3.3 \text{ ppm}\cdot\text{m}$  in 3.5 seconds was established. Dynamic concentration changes were detected, enabling the direct observation of turbulence in the release plume (Fig. 1). For tracking evaporation processes in the lab, a mixture of acetone, ethanol and alpha-pinene was used. The liquid mixture was placed in a 10 cm petri dish, under a 40 cm open-cell cavity (38.2 m effective path length). The system was able to detect the three compounds simultaneously and track the fluctuation of the vapor plume above the dish in real time. We achieved detection limits of  $\sim 50 \text{ ppm}\cdot\text{m}$ ,  $\sim 7 \text{ ppm}\cdot\text{m}$ , and  $\sim 2 \text{ ppm}\cdot\text{m}$  for acetone, ethanol and alpha-pinene, respectively, in 2.7 seconds. The two different applications both demonstrate the capability of the system in time-resolved measurement of gas concentration.



**Fig. 1** Results of the propane release experiment in the open-path configuration. (a) Retrieved concentration of propane at a time resolution of 128 ms (27 ms without integration). (b) Measured spectra (black) of red dot from (a) along with fitted spectra of propane (red) from PNNL database shown inverted, with fitting residual in the bottom panel. The featureless residual indicates a good fitting.

## References

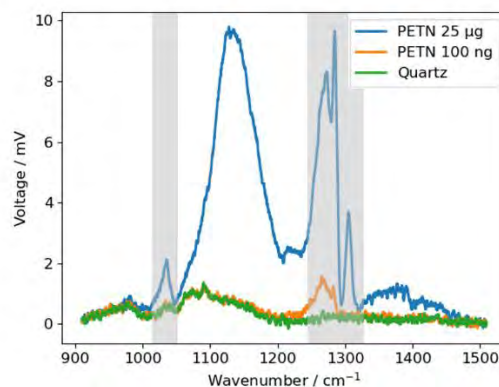
- [1] M. A. Abbas, K. E. Jahromi, M. Nematollahi, R. Krebbers, N. Liu, G. Woyessa, O. Bang, L. Huot, F. J. M. Harren, and A. Khodabakhsh, "Fourier transform spectrometer based on high-repetition-rate mid-infrared supercontinuum sources for trace gas detection," *Opt. Express* **29**, 22315-22330 (2021).
- [2] K. E. Jahromi, M. Nematollahi, R. Krebbers, M. A. Abbas, A. Khodabakhsh, and F. J. M. Harren, "Fourier transform and grating-based spectroscopy with a mid-infrared supercontinuum source for trace gas detection in fruit quality monitoring," *Opt. Express* **29**, 12381-12397 (2021).
- [3] K. E. Jahromi, Q. Pan, L. Høgstædt, S. M. M. Friis, A. Khodabakhsh, P. M. Moselund, and F. J. M. Harren, "Mid-Infrared Supercontinuum-Based Upconversion Detection for Trace Gas Sensing," *Opt. Express* **27**, 24469-24480 (2019).

# Sensitivity of a remote mid-infrared spectroscopy system for detecting traces of explosives

Lisa B. Dreier, Anja Köhntopp, Marc Steigleder, Christoph Geiß, Frank Duschek  
*German Aerospace Center, Institute of Technical Physics, Im Langen Grund 1, 74239 Hardthausen am Kocher*

**Short abstract:** Mid-infrared (MIR) spectroscopy is a promising technique for detecting traces of explosives in security applications. We investigate the sensitivity of a remote MIR detection system and discuss the resulting detection limit as well as data analysis strategies. Finally, we show first results for a detection algorithm for various explosive substances.

The detection of hazardous and illicit substances, such as explosives, plays a key role in security applications. The technologies that are currently being used for such applications are terahertz scanners, ion mobility spectrometry and mass spectrometry (swipe tests) and canines.[1,2] All of these technologies are either unable to detect traces of explosives or they require time consuming sampling and a lot of resources. Canines on the other hand are very sensitive and fast, but require frequent rests and training. All of those disadvantages may be overcome using mid-infrared (MIR) laser spectroscopy. MIR spectroscopy allows for contactless and fast detection of explosives. As the detection is based on molecular vibrations, the method is highly selective. We have developed a system that uses a quantum cascade laser (QCL) to detect traces of explosives at distances between 50 cm and 2 meters. A recent study investigated the sensitivity of our system for the explosives pentaerythritol tetranitrate (PETN), hexogen (RDX), trinitrotoluene (TNT) and ammoniumnitrate (AN) on quartz surfaces. The results clearly show that we are able to detect amounts well below 100 ng of the named explosives at a detection distance of 1 m. Figure 1 shows exemplary spectra of 25 µg and 100 ng of PETN on quartz as well as the bare quartz substrate for comparison. Clear PETN signals are visible at the highlighted spectral regions even at 100 ng. Here, we will discuss the detection limit of our system as well as data analysis strategies and a road toward a detection algorithm for these substances. Challenges that arise during the analysis of more complex substrates than quartz, such as textiles, will also be addressed.



**Fig. 1** MIR spectra of 25 µg and 100 ng PETN on quartz as well as a spectrum of the bare quartz substrate. The grey areas are a guide to the eye and mark the PETN signatures in the spectra.

## References

- [1] Glackin, J.M.E.; Gillanders, R.N.; Eriksson, F.; Fjällgren, M.; Engblom, J.; Mohammed, S.; Samuel, I.D.W.; Turnbull, G.A. "Explosives detection by swabbing for improvised explosive devices." *Analyst* 2020, **145**, 7956–7963.
- [2] Bauer, C.; Sharma, A.; Willer, U.; Burgmeier, J.; Braunschweig, B.; Schade, W.; Blaser, S.; Hvozدارa, L.; Müller, A.; Holl, G. Potentials and limits of mid-infrared laser spectroscopy for the detection of explosives. *Appl. Phys. B* 2008, **92**, 327–333



# Dual-Gas QEPAS based sensor for simultaneous detection of methane isotopologues

Mariagrazia Olivieri<sup>1</sup>, Arianna Elefante<sup>2</sup>, Giansergio Menduni<sup>1</sup>, Marilena Giglio<sup>1</sup>, Pietro Patimisco<sup>1,3</sup>, Vincenzo Spagnolo<sup>1,3</sup>, and Angelo Sampaolo<sup>1,3</sup>

<sup>1</sup> PolySense Lab, Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari, 70126 Italy

<sup>2</sup> Institute for Photonics and Nanotechnologies, CNR IFN, Via Amendola 173, 70126 Bari, Italy

<sup>3</sup> PolySense Innovations srl, Via Amendola 173, Bari, 70126 Italy

**Short abstract:** Two QCLs emitting at 7.83  $\mu\text{m}$  and 7.72  $\mu\text{m}$  were utilized to excite the fundamental and overtone modes of a spectrophone and simultaneously monitor the concentration of  $^{12}\text{CH}_4$  and  $^{13}\text{CH}_4$ . The sensor demonstrated the capability to detect ppm-level variations of  $^{13}\text{CH}_4$  within a matrix containing  $\text{CH}_4$  at percentage levels.

The possibility to accurately detect and quantify methane isotopologues, specifically  $^{12}\text{CH}_4$  and  $^{13}\text{CH}_4$ , is crucial to identify the origin of methane emissions, with applications in different fields such as climate research, environmental monitoring and petrochemical analysis [1]. Laser-based spectroscopic techniques have gained a crucial role in addressing these applications due to their high sensitivity, selectivity, and capability for real-time in situ detection. A crucial requirement for advanced isotopic sensing systems is the simultaneous detection of both isotopologues. Quartz-Enhanced Photoacoustic Spectroscopy-based multi-gas detection has been demonstrated in several studies, employing multiple laser sources or exploiting wide tuning ranges, but performing a sequential, non-simultaneous detection of different analytes. Wavelength Modulation Division Multiplexing (WMDM) has proven to be effective in achieving multiple-gas simultaneous detection. This approach is based on independent modulation of laser sources, each for a specific gas species, and simultaneous detection by means of a single detector. The development of custom QTFs capable of operating at both the fundamental and first overtone mode has paved the way for utilizing QEPAS technique in a WMDM configuration. Wu et al. presented a proof-of-concept for dual-gas QEPAS detection utilizing a custom QTF with a fundamental and overtone mode resonance frequency equal to 2.8 kHz and 17.78 kHz [2]. In the work proposed in [3], the same kind of custom QTF was used, acoustically coupled to two dual-tube acoustic resonators, to improve the signal-to-noise ratio of the sensor. Both studies demonstrated that the QEPAS signal at the QTF's fundamental frequency is unaffected by the overtone mode operation, and vice versa. The experimental setup is based on two DFB QCLs, emitting at 7.83  $\mu\text{m}$  and 7.72  $\mu\text{m}$ , to excite the QTF's fundamental and overtone modes and monitor the concentration of  $^{12}\text{CH}_4$  and  $^{13}\text{CH}_4$ , respectively. The sensor demonstrated the capability to analyse the isotopic composition of an unknown  $\text{CH}_4$  sample and with a detection limit in delta ratio assessment in the order of ‰ at  $\sim 1$  s integration time, within a matrix containing  $\text{CH}_4$  in natural abundance and at percentage levels.

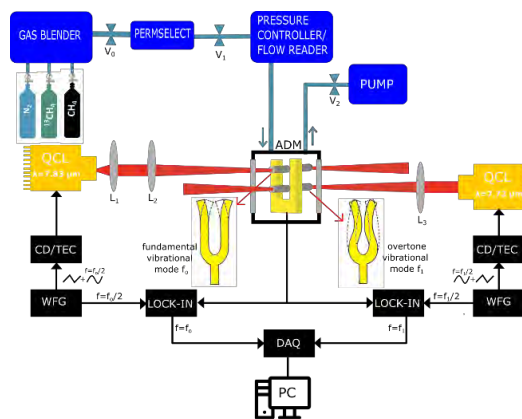


Fig. 1 Schematic of the experimental apparatus.

## References

- [1] B. B. Bernard, J. M. Brooks, and W. M. Sackett, "Natural gas seepage in the Gulf of Mexico," *Earth Planet. Sci. Lett.* 31(1), 48–54, Elsevier (1976).
- [2] H. Wu, X. Yin, L. Dong, K. Pei, A. Sampaolo, P. Patimisco, H. Zheng, W. Ma, L. Zhang, W. Yin, L. Xiao, V. Spagnolo, S. Jia, F.K. Tittel, Simultaneous dual-gas QEPAS detection based on a fundamental and overtone combined vibration of quartz tuning fork, *Cit. Appl. Phys. Lett.* 110, 121104 (2017).
- [3] A. Elefante, M. Giglio, A. Sampaolo, G. Menduni, P. Patimisco, V.M.N. Passaro, H. Wu, H. Rossmadl, V. Mackowiak, A. Cable, F.K. Tittel, L. Dong, V. Spagnolo, "Dual-gas quartz-enhanced photoacoustic sensor for simultaneous detection of methane/nitrous oxide and water vapor." *Analytical chemistry* 91.20 (2019): 12866-12873.

# Multigas simultaneous detection based on photoacoustic spectroscopy technology

Hongpeng Wu<sup>1,2</sup>, Chaofeng Sun<sup>1,2</sup>, Xiaowen Shen<sup>1,2</sup>, Ruyue Cui<sup>1,2</sup> and Lei Dong<sup>1,2</sup>

1. State Key Laboratory of Quantum Optics Technologies and Devices, Institute of Laser Spectroscopy, Shanxi University, Taiyuan 030006, China

2. Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan 030006, China

**Short abstract:** Photoacoustic spectroscopy (PAS), known for its advantages of excellent selectivity, high detection precision, and long lifespan, has long been a focal point of research. This paper proposes the use of a photoacoustic cell for simultaneous multi-gas detection. The photoacoustic cell is designed with multiple resonant cavities that have base frequencies that are close yet distinct. By employing frequency division multiplexing, the system achieves the simultaneous detection of multiple gases.

Trace gas sensing technology based on photoacoustic spectroscopy is widely applied in various fields such as environmental pollution, aerospace, and biomedical sciences[1]. In 1938, Viengerov introduced a photoacoustic (PA) system that utilized a blackbody infrared source and a microphone for the analysis of gas mixtures. In the 1960s, a significant breakthrough occurred with the first use of a laser light source in PA gas detection. However in a conventional PAS configuration, a single acoustic resonator operates at its own resonant frequency, making it challenging to simultaneously capture the photoacoustic signals from different lasers for multi-component analysis. In this paper, we propose the design of multiple resonant cavities for the simultaneous detection of multiple gas components. We have developed a photoacoustic cell consisting of three acoustic resonators with distinct resonant modes, and a single microphone is used to simultaneously detect the photoacoustic signals from each resonator[2]. Figure 1 shows the simulation of the acoustic pressure distribution in the three resonant cavities of the designed photoacoustic cell at different frequencies, using COMSOL Multiphysics software.



**Fig. 1** Simulation of the acoustic pressure in the three resonant cavities at different frequencies.

The photoacoustic cell consists of three cylindrical acoustic resonators, each with a specific length, providing distinct acoustic resonant frequencies. From the simulation results, we identified the optimal resonant frequencies for the three resonators as  $f_0 = 1320.1$  Hz,  $f_1 = 1398.6$  Hz, and  $f_2 = 1509.1$  Hz. These values correspond to the first longitudinal resonant mode of each resonator. We will use this design for simultaneous multi-gas detection by modulating the laser at these three frequencies. This design allows a single microphone to detect the PAS signals from each resonator, utilizing second-harmonic modulation-demodulation technology, and the signals from each resonator are demodulated at their respective resonant frequencies using a lock-in amplifier.

In conclusion, this design has broad application potential for simultaneous detection of multi-component gases. Furthermore, we can design photoacoustic cells with more resonant cavities at different frequencies to enable the simultaneous detection of additional gases.

## References

- [1] H. Wu, L. Dong, H. Zheng, Y. Yu, W. Ma, L. Zhang, W. Yin, L. Xiao, S. Jia and F. K. Tittel, "Beat frequency quartz-enhanced photoacoustic spectroscopy for fast and calibration-free continuous trace-gas monitoring," Nat. Commun. 8, 15331 (2017).
- [2] Kun Liu, Jiaoxu Mei, Weijun Zhang, Weidong Chen, Xiaoming Gao, Multi-resonator photoacoustic spectroscopy, Sensors and Actuators B: Chemical, Volume 251, (2017).

# Spectroscopy for air pollutants detection - Sponsored by Project MAECI



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# Remote sensing of vertical distribution of greenhouse gases in the atmospheric column using laser heterodyne radiometer

Aditya Saxena<sup>1</sup>, Yongyong Hu<sup>1</sup>, Tingting Wei<sup>1</sup>, Jingjing Wang<sup>1,2</sup>, Fengjiao Shen<sup>1</sup>, Tu Tan<sup>2</sup>, Marie Thérèse El Kattar<sup>1</sup>, Mélanie Ghysels-Dubois<sup>3</sup>, Hervé Herbin<sup>4</sup>, Weidong Chen<sup>1</sup>

1. Laboratoire de PhysicoChimie de l'Atmosphère (LPCA), Université du Littoral Côte d'Opale, Dunkerque, France

2. Anhui Institute of Optics and Fine Mechanics (AIOFM), Chinese Academy of Sciences, Hefei, China

3. Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA), Université de Reims, UMR 7331 CNRS, Reims, France

4. Laboratoire d'Optique Atmosphérique (LOA), Université de Lille, UMR 8518 CNRS, Lille, France

**Short abstract:** Development and application of laser heterodyne radiometer for remote sensing of greenhouse gases (GHGs) concentration distribution in the atmospheric column will be presented. Intercomparisons with other in-situ and ground-based measurements show its high potential for worldwide network measurement of vertical concentration profile of GHGs in the atmosphere.

Vertical concentration distribution of atmospheric trace gases, depending on vertical air transport from the Earth's surface to the tropopause, play crucial roles in air pollution, ozone depletion and climate change. The accurate determination of vertical concentration profile of greenhouse gases (GHGs) in the atmospheric column is important in the current international context of fighting against global warming and climate change. Laser heterodyne radiometry technique, which extracts target molecular absorption information from the broadband sunlight by beating it with a local oscillator for heterodyne measurement, is a highly effective method for the precise measurement of GHGs' concentration and vertical profile in the atmospheric column [1].

A transportable, all-fiber-coupled laser heterodyne radiometer (LHR) has been developed for ground-based remote sensing of carbon dioxide (CO<sub>2</sub>) [2,3], water vapor (H<sub>2</sub>O) and methane (CH<sub>4</sub>) in the atmospheric column by using a wide band tunable external-cavity diode laser (1520 – 1620 nm) as local oscillator.

The LHR performance, as well as the data analysis and data inversion has been performed using ARAHMIS (Atmospheric Radiation Algorithm for High-Spectral Resolution Measurements from Infrared Spectrometers) [4].

LHR instrument configuration and experiment detail, as well as the performance intercomparison results will be presented.

## Acknowledgments

This work is partially supported by the French national research agency (ANR) under the Labex CaPPA (ANR-10-LABX-005) contract, the EU H2020-ATMOS project (Marie Skłodowska-Curie grant agreement No 872081), the regional CPER ECRIN program, and the CNES ATMOSFER project.

## References

- [1] D. Weidmann, "Atmospheric trace gas measurements using laser heterodyne spectroscopy", Ch. 4, pp. 159-223, in *Advances in Spectroscopic Monitoring of the Atmosphere*, eds. by Weidong Chen, Dean S. Venables, Markus W. Sigrist, ISBN: 978-0-12-815014-6, Elsevier (2021).
- [2] J. Wang, T. Tu, F. Zhang, F. Shen, J. Xu, Z. Cao, X. Gao, S. Plus, and W. Chen, "An external-cavity diode laser-based near-infrared broadband laser heterodyne radiometer for remote sensing of atmospheric CO<sub>2</sub>", *Optics Express* **31** (2023) 9251-9263.
- [3] M. T. El Kattar, T. Wei, A. Saxena, H. Herbin, and W. Chen, "Potential CO<sub>2</sub> measurement capabilities of a transportable near infrared laser heterodyne radiometer (LHR)", *Atmos. Meas. Tech.* (2025), egusphere-2025-250, <https://doi.org/10.5194/egusphere-2025-250>
- [4] M.T. El Kattar, F. Auriol, H. Herbin, "Instrumental Characteristics and potential greenhouse gas measurement capabilities of the Compact High-Spectral-Resolution Infrared spectrometer: CHRIS", *Atmospheric Measurement Technique* **13** (2020) 3769-3786.

# The Sky's the Limit: Compact Trace Gas Sensors for Airborne Explorations

Béla Tuzson<sup>1</sup>, Simone Brunamonti<sup>1</sup>, Philipp Scheidegger<sup>1,2</sup>, André Kupferschmid<sup>2</sup>, Herbert Looser<sup>1</sup>,  
Timo Kaldewey<sup>1</sup>, Lorenz Heilmann<sup>1</sup>, Alex Weitnauer<sup>1,3</sup>, and Lukas Emmenegger<sup>1</sup>

1. Empa, Laboratory for Air Pollution / Environmental Technology, 8600, Dübendorf, Switzerland

2. Empa, Transport at Nanoscale Interfaces Laboratory, 8600, Dübendorf, Switzerland

3. ETH, Institute for Atmospheric and Climate Science, 8093, Zürich, Switzerland

**Short abstract:** Recent innovations of key components have enabled the development of portable laser spectrometers with a compact "shoebox" design. These robust, high-precision devices can provide real-time, high-resolution data for urban, industrial, and atmospheric monitoring, even in harsh environments.

Laser absorption spectroscopy is a proven technology for reliable and high-precision gas sensing. With the advent of state-of-the-art laser sources, a wide variety of analytical techniques have been developed, significantly extending applications beyond the laboratory environment. Yet, full portability and downscaling has remained a significant challenge, particularly when maintaining selectivity, sensitivity, and precision.

In this presentation, we address this challenge and highlight some of our ongoing developments of key technologies that have contributed to enable the realization of high-precision portable spectrometers with a "shoebox" footprint, i.e., weighing below 4 kg and consuming less than 20 W of power. These developments include a robust and lightweight circular segmented multipass cell [1], the concept of low-heat-dissipation intermittent-continuous-wave (iCW) laser driving, and FPGA-based electronics for fast data acquisition and processing [2]. Merging these key improvements resulted in fully autonomous devices characterized by exceptional robustness, compactness, rigidity, and high sensitivity, which can be seamlessly integrated into flying platforms. This creates new opportunities for applications requiring high spatio-temporal resolution, such as urban or industrial site monitoring and upper atmosphere observation. We will review some illustrative examples [3–5] of our exploratory missions to demonstrate their airborne capability of capturing subtle and/or sudden changes in atmospheric trace gas concentrations and providing real-time data with 1-second time resolution and outstanding precision, even under harsh environmental conditions.

These innovations promise transformative applications in environmental monitoring offering real-time, high-resolution data from hard to access locations.

## References

- [1] M. Graf, L. Emmenegger, and B. Tuzson, "Compact, circular, and optically stable multipass cell for mobile laser absorption spectroscopy," *Opt. Lett.* **43**, 2434–2437 (2018).
- [2] C. Liu, B. Tuzson, P. Scheidegger, H. Looser, B. Bereiter, M. Graf, M. Hundt, O. Aseev, D. Maas, and L. Emmenegger, "Laser driving and data processing concept for mobile trace gas sensing: Design and implementation", *Rev. Sci. Instrum.* **89** (6), 065107 (2018).
- [3] B. Tuzson, M. Graf, J. Ravelid, P. Scheidegger, A. Kupferschmid, H. Looser, R. P. Morales, and L. Emmenegger, "A compact QCL spectrometer for mobile, high-precision methane sensing aboard drones", *Atmos. Meas. Tech.* **13**, 4715–4726, (2020).
- [4] M. Graf, P. Scheidegger, A. Kupferschmid, H. Looser, T. Peter, R. Dirksen, L. Emmenegger, and B. Tuzson, "Compact and lightweight mid-infrared laser spectrometer for balloon-borne water vapor measurements in the UTLS", *Atmos. Meas. Tech.* **14**, 1365–1378, (2021).
- [5] S. Brunamonti, M. Graf, T. Bühlmann, C. Pascale, I. Ilak, L. Emmenegger, and B. Tuzson, "SI-traceable validation of a laser spectrometer for balloon-borne measurements of water vapor in the upper atmosphere", *Atmos. Meas. Tech.* **16**, 4391–4407, (2023).



# Laser-wavelength-tuned CRDS for real-time measurement of trace gas

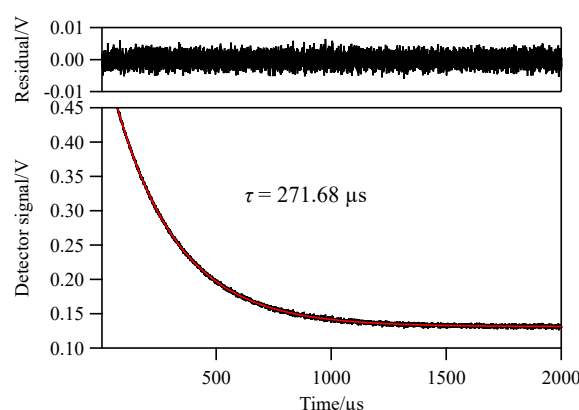
Hisashi Abe<sup>1</sup>

*1. National Metrology Institute of Japan (NMIJ), AIST Tsukuba Central 3, Tsukuba 305-8563, Japan*

**Short abstract:** A relatively simple technique for laser control and coupling a laser frequency to a cavity mode for CRDS was developed. The laser wavelength is tuned to the center of an absorption line of the target gas (water vapor), and the resonant frequencies of the cavity are modulated using a piezoelectric element.

Cavity Ring-Down Spectroscopy (CRDS) is a powerful technique for measuring trace species in the gas phase, particularly for trace amounts of water vapor (trace moisture) [1]. By using a high finesse optical resonator (optical cavity), an effective optical path length of several kilometers or more can be easily achieved, enabling high sensitivity. Furthermore, the absolute value of the absorption coefficient can be obtained, allowing quantitative measurements without the use of a standard gas for the calibration. In CRDS, the frequency of the probe laser must be coupled to a resonance frequency of the cavity (a cavity mode). For accurate control of both the probe laser and resonant frequencies, various techniques have been developed such as comb-locked CRDS [2], which requires advanced laser control techniques using optical frequency comb, Pound-Drever-Hall technique, high-performance electronics for high-speed locking, and so on. In this study, I developed a relatively simple technique for laser control and frequency coupling, referred to as “laser-wavelength-tuned CRDS.” In this technique, the laser wavelength is tuned to the center of an absorption line of the target gas (water vapor in this study), and the resonant frequencies are modulated to much the laser frequency. By measuring ring-down time ( $\tau$ ) only at the center position rather than recording a spectrum over the absorption line, this approach enables more effective data acquisition for determining the water concentration. In addition, it can determine the water concentration only using a simple formula without any spectral analysis, which should be suitable for real-time measurement.

An optical cavity made of stainless steel with a cavity length of 60 cm was constructed using two highly reflective mirrors with a reflectivity of 99.9993 % at a wavelength of 1.393  $\mu\text{m}$ . The cavity length was modulated by approximately 0.7  $\mu\text{m}$  (corresponding to half a wavelength of the probe laser) using a piezoelectric element introduced inside the mirror mount on one side. The wavelength of a DFB laser was measured with a wavelength meter, and the driving current of the DFB laser was PID-controlled to tune the laser frequency to the center of the absorption line (7181.145  $\text{cm}^{-1}$ ) of water in nitrogen at 1 atm using the built-in function of the wavelength meter. Figure 1 shows an example of  $\tau$  measurement by introducing dry nitrogen into the cavity with a residual water content of about 2 nmol/mol (2 ppb) in mole fraction. Fitting with an exponential function resulted in  $\tau = 271.68 \mu\text{s}$ . The detection sensitivity (standard deviation) for trace moisture was estimated to be 0.15 nmol/mol (0.15 ppb) with an integration time of 1 s. The measurement uncertainty evaluated from the comparison with a primary trace-moisture standard at National Metrology Institute of Japan as well as the results of the real-time measurement will be presented.



**Fig. 1** Ring-down time measurement at the center of a water absorption line using laser-wavelength-tuned CRDS.

This study was supported in part by JST, CREST Grant Number JPMJCR2104, Japan.

## References

- [1] H. Abe, “Trace-moisture measurement using cavity ring-down spectroscopy at NMIJ,” *Journal of Physics: Conference Series* **2439**, 012001 (2023).
- [2] A. Castrillo, M. A. Khan, E. Fasci, V. D’Agostino, S. Gravina, L. Gianfrani, “Demonstration of record sensitivity for water vapor detection by means of comb-locked cavity ring-down spectroscopy,” *Optica* **11**, 1277 (2024).

# An open-path observatory for greenhouse gases using dual comb spectroscopy

Schmitt Tobias D.<sup>1</sup>, Dubroeuq Romain<sup>1,2</sup>, Sindram Moritz<sup>3</sup>, Pfeifer Thomas<sup>2</sup>, Butz André<sup>3,4,5</sup>, Oberthaler Markus K.<sup>1</sup>

1. Kirchhoff-Institute for Physics (KIP), Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg – Germany

2. Max-Planck Institute for Nuclear Physics (MPIK), Saupfercheckweg 1, 69117 Heidelberg – Germany

3. Institute of Environmental Physics (IUP), Heidelberg University, Im Neuenheimer Feld 229, 69120 Heidelberg – Germany

4. Heidelberg Center for the Environment (HCE), Heidelberg University, Im Neuenheimer Feld 130.1, 69120 Heidelberg – Germany

5. Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University, Im Neuenheimer Feld 205, 69120 Heidelberg – Germany

**Short abstract:** We present the setup of a near-infrared dual comb spectrometer for open-path measurements of greenhouse gases over the city of Heidelberg and the results of its first deployment in a side-by-side measurement with a Fourier transform spectrometer.

Urban areas are a major and growing contributor to anthropogenic greenhouse gas (GHG) emissions, but their contribution is also subject to significant uncertainty [1]. Measurement-based information of these emissions is rarely available to policymakers, but could facilitate more informed planning, implementation, and monitoring of emission-reduction efforts. But the heterogeneous emission landscapes of urban areas pose a significant challenge for measurement-based estimations of these emissions. These estimation methods typically combine atmospheric transport models on the kilometer scale with measurements of GHG concentrations by point-like in-situ sensors, which are highly sensitive to local influences and not necessarily representative on the kilometer scale. Thus, path-averaged measurements of GHG concentrations are of interest to analyze and potentially to overcome these issues of representativeness.

In principle, many spectroscopic techniques are suited for these measurements, but methods with a broad spectral coverage are preferable – not only because they can cover multiple species simultaneously, but also because accessing full rotation-vibration bands provides a constraint on the average temperature of the airmass, which is not necessarily available otherwise. Traditional Fourier transform infrared (FTIR) spectroscopy fulfills these requirements [2]. It can also perform these measurements at resolutions higher than the linewidths of the collision-broadened absorption lines [3], but lacks in sensitivity due to limited brightness of thermal light sources. Frequency comb techniques can overcome this limitation by providing a bright, coherent, and broadband light source. Among frequency comb techniques, dual comb spectroscopy (DCS) is particularly suited for remote sensing and field deployment outside optical laboratories, since it allows for compact and mechanically robust instrument design [4]. High costs and the experience required to set up and operate such a system limits the application to metrology experts, but with the increasing commercial availability of turn-key frequency combs, DCS becomes a more realistic option for a wider scientific community.

We present the development of a near-infrared dual comb spectrometer for open-path measurements of GHG concentrations above the city of Heidelberg and the results of its first deployment along a 1.55 km atmospheric path. The core of the system are two fully stabilized commercially available turn-key frequency combs. A single telescope sends and receives the combined light to and from an array of retro reflectors, resulting in a 3.1 km long absorption path. We discuss the results and performances during the first deployment of the system and compare them to a co-deployed FTIR instrument.

## References

- [1] Federal Environment Agency, "National Inventory Report for the German Greenhouse Gas Inventory 1990 – 2019" UNFCCC Submission (2021)
- [2] D. W. T. Griffith, D. Pöhler, S. Schmitt, S. Hammer, S. N. Vardag, and U. Platt "Long open-path measurements of greenhouse gases in air using near-infrared Fourier transform spectroscopy" *Atmos. Meas. Tech.*, **11**, 1549-1563 (2018)
- [3] T. D. Schmitt, J. Kuhn, R. Kleinschek, B. A. Löw, S. Schmitt, W. Cranton, M. Schmidt, S. N. Vardag, F. Hase, D. W. T. Griffith, and A. Butz "An open-path observatory for greenhouse gases based on near-infrared Fourier transform spectroscopy" *Atmos. Meas. Tech.*, **16**, 6097-6110 (2023)
- [4] G. B. Rieger, F. R. Giorgetta, W. C. Swann, J. Kofler, A. M. Zolot, L. C. Sinclair, E. Baumann, C. Cromer, G. Petron, C. Sweeney, P. P. Tans, I. Coddington, and N. R. Newbury "Frequency-comb-based remote sensing of greenhouse gases over kilometer air paths" *Optica* **1**(5), 290-298 (2014)

## Laser Heterodyne Radiometry: Applications from Solar Occultation to Wildfire Characterization

J. Houston Miller<sup>1</sup>, Monica Flores<sup>1,2</sup>, Erin McCaughey<sup>1</sup>, David Bomse<sup>3,4</sup>

<sup>1</sup>Department of Chemistry, George Washington University, Washington, DC 20052 USA

<sup>2</sup>Current position: US National Institute of Standards and Technology

<sup>3</sup>Mesa Photonics, 1550 Pacheco Street, Santa Fe, NM 87505 USA

<sup>4</sup>Current position: retired

Optical heterodyne methods are like their electronic counterparts used in radio and television, among other applications. Incoming light is combined with light from a narrow-band laser source (the local oscillator or LO) on a photodetector. Historically, most applications of LHR have focused on solar occultation spectroscopy and its development has tracked the availability of (and improvements in) low-noise laser sources and detectors. The GW Laser Analytics group (GWLAG) has participated in the development of Laser Heterodyne Radiometry (LHR) instruments in conjunction with NASA Goddard and more recently through a partnership with Mesa Photonics. Our LHR work includes both aspects of instrument design and control and retrieval of species concentrations from measured column spectra.

For the past year, we have focused on the development and demonstration of a LHR instrument for wildfire detection and characterization. We are building two sensor platforms for laboratory measurements as well as simple “field-scale” demonstrations. The first system will operate in the near-infrared spectral region ( $\sim 0.77\ \mu\text{m}$ ) and will focus on potassium detection. (Light emission from hot potassium ions is a characteristic of only intense fires of plant materials and not fossil fuels.) The second system will be constructed for operation at  $4.55\ \mu\text{m}$  and will focus on detection of both carbon monoxide and carbon dioxide radiative emissions. These two molecules can be used to estimate combustion efficiency: the percentage of carbon emissions from a flame that is carbon dioxide.

This presentation will introduce Laser Heterodyne Radiometry, summarize our solar occultation work, and provide a progress report on LHR application to combustion and fire measurements.

# Assessment of N<sub>2</sub>O emissions from soil using a portable photoacoustic spectroscopy system

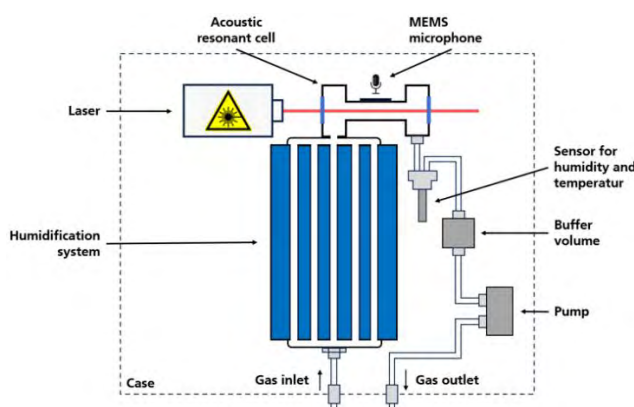
Gerrit Stiefvater<sup>1,2</sup>, Raimund Brunner<sup>1</sup>, Miguel Hamburger<sup>1</sup>, Tobias Kolleth<sup>1</sup>, Sven Rademacher<sup>1</sup>, Thomas Strahl<sup>1,2</sup>, Jürgen Wöllenstein<sup>1,2</sup>

1. Fraunhofer Institute for Physical Measurement Techniques IPM, Georges-Köhler-Allee 301, 79110 Freiburg – Germany

2. University of Freiburg, IMTEK, Laboratory for Gassensors, Georges-Köhler-Allee 102, 79110 Freiburg - Germany

**Short abstract:** A portable photoacoustic sensing system for N<sub>2</sub>O soil emissions in agriculture is presented. The focus was on developing a temperature-stabilized humidification system for gas conditioning within the sampling system to enable precise N<sub>2</sub>O concentration deviations above the ambient air concentration of 335 ppb.

Measuring nitrous oxide (N<sub>2</sub>O), also known as laughing gas, is important in various applications, including agriculture. During fertilisation, some of the nitrogen in the soil that is not required by the plants is converted into N<sub>2</sub>O. Measuring N<sub>2</sub>O helps to understand complex processes in the soil and thus enables targeted, efficient fertilisation. This will save valuable fertiliser resources, reduce emissions of N<sub>2</sub>O as a greenhouse gas with a greenhouse potential of 273, and prevent nitrate pollution in the soil [1]. To resolve the very low N<sub>2</sub>O soil emissions (< 10 µg / (m<sup>2</sup> min)), it is necessary to measure the N<sub>2</sub>O concentration deviation above the ambient air concentration of 335 ppb with a high accuracy and precision (e.g. 5 ppb). This study presents a novel approach for the precise measurement of N<sub>2</sub>O emissions from the soil using photoacoustic spectroscopy (PAS) combined with an innovative sampling system.



**Fig. 1** Schematic setup of the gas circuit in the measuring case including PAS and humidification system (left). Measuring system and N<sub>2</sub>O sampling hoods in the field test (right).

PAS enables a compact configuration of the measurement system's optics and high sensitivity [2]. Furthermore, the integration of a cutting-edge interband cascade laser (ICL), characterised by its minimal power requirements, ensures battery-powered operation, thereby enabling portability within field applications. Equipped with a replaceable 12,000 mAh rechargeable battery, 5 h of measurement is possible. With this PAS setup, N<sub>2</sub>O is measured in the mid-infrared using an ICL with a wavelength of 4.5 µm. In terms of the photoacoustic signal generation, a humidification system has been installed (see Fig. 1). In combination with thermal management, the humidification system maintains a consistently high humidity level in the gas sample in order to provide a high accuracy and precision. Furthermore, the temperature-stabilized humidification system is a key to minimise the influence of humidity and temperature effects on the gas sample.

A sophisticated sampling procedure allows to capture N<sub>2</sub>O emissions from the soil. The configuration is crucial to reduce potential influencing factors such as heating and changes in humidity within the hood, pressure differences during gas exchange or disturbances in soil physiology. The accumulated N<sub>2</sub>O concentration is measured on-site in the field while the gas sample circulates between the sampling hoods and the measuring cell. Ultimately, a precision better than 5 ppb at an averaging time of 5 s is achieved. This makes it possible to reliably assess the N<sub>2</sub>O emissions from soil with this portable photoacoustic measurement device.

## References

- [1] M. Zaman et al., *Measuring Emission of Agricultural Greenhouse Gases and Developing Mitigation Options Using Nuclear and Related Techniques*, Springer, ISBN 978-3-030-55395-1 (2021).
- [2] K. Schmitt, M. Sendelbach, C. Weber, J. Wöllenstein, and T. Strahl, "Resonant photoacoustic cells for laser-based methane detection," *J. Sens. Sens. Syst.*, **12**, 37–44, (2023)

# Poster Session



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# Simple cross-comb spectroscopy with a dual-comb optical parametric oscillator and real-time coherent averaging

C. P. Bauer<sup>1,2</sup>, L. Lang<sup>1</sup>, J. Pupeikis<sup>1</sup>, B. Willenberg<sup>1</sup>, L. Emmenegger<sup>2</sup>, B. Tuzson<sup>2</sup>, U. Keller<sup>1</sup>

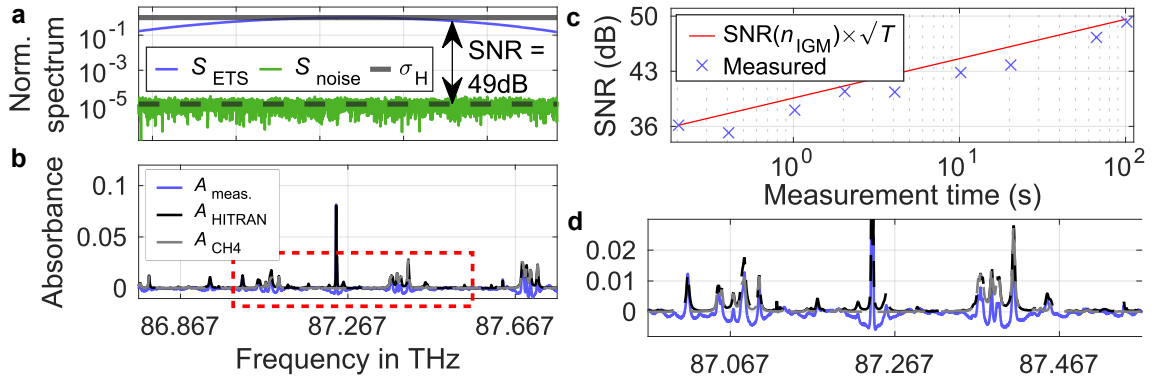
1. Institute for Quantum Electronics, ETH Zurich, Auguste-Piccard Hof 1, 8093 Zurich, Switzerland

2. Laboratory for Air Pollution / Environmental Technology, EMPA, Dübendorf, 8600, Switzerland

**Short abstract:** We employ a 250-MHz synchronously-pumped single-cavity dual-comb optical parametric oscillator in a simple cross-comb spectroscopy detection scheme with a 36-m multipass cell. We achieve a signal-to-noise-ratio of 38 dB Hz<sup>1/2</sup> and 49 dB after coherently averaging for 100 s in real-time. In a proof-of-concept measurement, we detect ambient methane.

Dual-comb spectroscopy (DCS) enables rapid high-resolution gas measurements across wide spectral ranges [1] and has proven to be a powerful tool for quantifying greenhouse gases in the atmosphere. However, achieving optimal measurement sensitivity to reduce the measurement time or the integration path length remains a challenge. Synchronously pumped optical parametric oscillators (OPOs) are an ideal source to access the mid-infrared, given their wide tunability, high conversion efficiencies, and the preservation of the low noise performance of the pump. In addition, a dual-comb OPO can be leveraged as a spectroscopic transceiver in a cross-comb spectroscopy (CCS) detection scheme, where in a recent demonstration, ultra-high sensitivity in the mid-infrared (signal-to-noise-ratio (SNR) >50 dB Hz<sup>1/2</sup> [2]) has been demonstrated.

In this work, we demonstrate a simplified version of CCS compared to ref. [2], while applying real-time coherent averaging and a 36-m long multipass cell (Aerodyne) filled with ambient air. The OPO is implemented in a rigid aluminum housing to reduce its susceptibility to environmental noise sources. This allows direct tracking of the idler phase such that only one photodiode is required. In addition, we avoid saturation of the photodiode and thus the necessity to stitch a saturated and non-saturated trace to reconstruct the trace's timing information. Hence, the computational effort is heavily reduced allowing real-time coherent averaging using a 16-bit data acquisition card (M4i.4451-x8, Spectrum Instrumentation).



**Fig. 1** (a) Coherently-averaged 100-s-long CCS measurement of ambient air over a total path length of 40 m. Measured spectrum  $S_{ETS}$  (blue), measured noise floor  $S_{noise}$  (green). (b) Comparison of the predicted absorbance based on HITRAN data for  $H_2O$  and  $CH_4$  (black),  $CH_4$  contribution only (grey), and the measured absorbance (blue), where etalons are removed in post-processing. (c) SNR as a function of the measurement time  $T$  (blue crosses), compared to the SNR of a 0.25-s long measurement scaled with  $\sqrt{T}$  (red). (d) Zoom in to (b) as indicated by the red mark.

At a center wavelength of 3.44  $\mu m$  ( $\nu_0 = 87$  THz,  $\Delta\nu_{FWHM} = 0.65$  THz), we obtain a high SNR of 38 dB Hz<sup>1/2</sup> (Fig. 1a) and can coherently average for more than 100 s (Fig. 1c). In a proof-of-concept measurement, we detect ambient methane ( $CH_4$ ) with a concentration of 1.5 ppm (Fig. 1b, d). To improve the residuals, a reference measurement on an emptied cell can be used to extract the spectrum's envelope. In a next step, we apply the system to trace gas detection.

**Authors declarations.** The presented work is the result of a collaboration between ETH and EMPA.

## References

- [1] I. Coddington, N. Newbury, and W. Swann, "Dual-comb spectroscopy," *Optica* **3**, 414-426 (2016).
- [2] C. P. Bauer, Z. A. Bejm, M. K. Bollier, J. Pupeikis, B. Willenberg, U. Keller, and C. R. Phillips, "High-sensitivity dual-comb and cross-comb spectroscopy across the infrared using a widely tunable and free-running optical parametric oscillator," *Nat. Commun.* **15**, 7211 (2024).

# Dual Laser diode integration in a silicon duplexers for multi-gas spectroscopy

Gabriele Biagi<sup>1,2</sup>, Ajmal Thottoli<sup>1,3</sup>, Artem Vorobev<sup>1</sup>, Petr Záruba<sup>4</sup>, Maria Kotlyar<sup>1</sup>, Liam O’Faolain<sup>1</sup>

<sup>1</sup>Centre for Advanced Photonics & Process Analysis, Munster Technological University, Cork, Ireland

<sup>2</sup>PolySenSe Lab - Dipartimento Interateneo di Fisica, Polytechnic and University of Bari, Bari, Italy

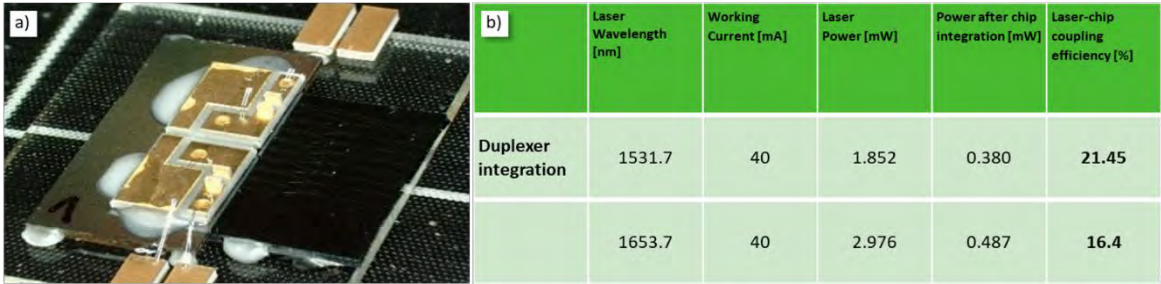
<sup>3</sup>Polytechnic University of Bari, Via E. Orabona, 4, Bari, Italy

<sup>4</sup>Argotech a.s., Trutnov, Czech Republic

**Short abstract:** The integration of two laser diodes using a silicon nitride directional coupler-based duplexers is proposed to achieve a compact (2 cm by 2.5 cm) source for a multi-gas spectroscopy. The developed device demonstrates potential for simultaneous detection of ammonia and methane, offering a promising solution for portable environmental monitoring applications.

Methane (CH<sub>4</sub>) is one of the major greenhouse gases produced in Europe, with agriculture contributing approximately 56% of total emissions, primarily due to enteric fermentation in ruminant livestock. Other notable sources include waste disposal, industries, and oil/gas mining [1-2]. On the other hand, ammonia (NH<sub>3</sub>) is widely used in the agriculture sector due to its critical role as a fertilizer component, enhancing plant growth and crop yields [3].

Among the various strategies that have been explored to enable multi-gas detection in spectroscopy-based systems, a widely adopted method involves the use of laser sources capable of addressing multiple absorption features, such as frequency combs, QCL arrays, or external cavity QCLs [4-5]. An alternative approach is to employ fiber combiners or optical components such as lenses and mirrors to couple multiple lasers, each targeting a different absorption feature [6-7]. While fiber-based delivery can mitigate alignment issues and achieve high detection sensitivity, it lacks the compactness and integration required for portable or field applications. In this work, we present the integration of two laser diodes using a silicon nitride directional coupler (DC)-based duplexers (Fig. 1a), designed to operate in the near-infrared (NIR) spectral region.



**Fig.1** (a) Microscope image of the multi-laser device. (b) Comparison of the output optical powers at different stages of integration.

The selected laser diodes target the absorption features of ammonia and methane at 1531.6 nm and 1653.7 nm, respectively. The duplexers was optimized to achieve coupling efficiencies of 80% and 83% within a 7 mm × 7 mm silicon chip footprint. The duplexers employs a 300 nm layer of silicon nitride (Si<sub>3</sub>N<sub>4</sub>) covered by a 1 μm-thick silicon oxide (SiO<sub>2</sub>) layer for guiding elements. The detected power values for the different stages are shown in Fig. 1b. The achieved output powers, along with the compact footprint, make the system well-suited for multi-gas detection using Tunable Diode Laser Absorption Spectroscopy (TDLAS) and Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) techniques.

## References

[1] EEA/PUBL/2024/046, “Annual European Union greenhouse gas inventory 1990–2022 and inventory document 2024”, 13 Dec (2024).  
[2] EEA Briefing No 01/2025, “Methane, climate change and air quality in Europe: exploring the connections”, doi: 10.2800/0096912, (2025).  
[3] The Royal Society, “Ammonia: zero-carbon fertiliser, fuel and energy store”, <https://royalsociety.org/-/media/policy/projects/green-ammonia/green-ammonia-policy-briefing.pdf>, (2020).  
[4] Picqué, N., Hänsch, T.W. Frequency comb spectroscopy. *Nature Photon* **13**, (146–157), (2019).  
[5] A. Zifarelli et al., “Multi-gas quartz-enhanced photoacoustic sensor for environmental monitoring exploiting a Vernier effect-based quantum cascade laser,” *Photoacoustics*, vol. **28**, (p. 100401), Dec. (2022), doi: 10.1016/j.pacs.2022.100401.  
[6] Menduni et al., “Fiber-Coupled Quartz-Enhanced Photoacoustic Spectroscopy System for Methane and Ethane Monitoring in the Near-Infrared Spectral Range,” *Molecules*, vol. **25**, no. 23, (p. 5607), Nov. (2020), doi: 10.3390/molecules25235607.  
[7] P. Patimisco et al., “Quartz-Enhanced Photoacoustic Sensor Based on a Multi-Laser Source for In-Sequence Detection of NO<sub>2</sub>, SO<sub>2</sub>, and NH<sub>3</sub>,” *Sensors*, vol. **23**, no. 21, (p. 9005), Nov. (2023), doi: 10.3390/s23219005.

# Mapping of CH<sub>4</sub> atmospheric plumes from point sources by open -path TDLAS and AI-assisted tomographic reconstruction: numerical proof of concept

Claire Birot<sup>1</sup>, Gautier Vilmar<sup>1</sup>, Myriam Raybaut<sup>1</sup>, Frédéric Champagnat<sup>2</sup>, Grégoire Broquet<sup>3</sup>, Pramod Kumar<sup>3</sup>, Christophe Brossard<sup>1</sup>, Aurélien Plyer<sup>2</sup>

1. DPHY, ONERA, Université Paris-Saclay, 91120, Palaiseau, France

2. DTIS, ONERA, Université Paris-Saclay, 91120, Palaiseau, France

3. Laboratoire des Sciences du Climat et de l'Environnement (LSCE/IPSL), CEA-CNRS-UVSQ, Université Paris Saclay, 91191 Gif-sur-Yvette, France

**Short abstract:** Tomographic reconstruction for CH<sub>4</sub> releases from point sources is studied to locate and cartography a leak from non-intrusive synthetic measurements which could be obtained by tunable diode laser absorption spectroscopy.

Optical diagnostics, such as Tunable Diode Laser Absorption Spectroscopy (TDLAS), are commonly used to measure concentration in a non-intrusive-way. One possible application is the detection and quantification of gas into the atmosphere, such as CH<sub>4</sub> leaks from industrial sites and facilities. However, TDLAS technique does not allow the retrieval of the spatial distribution of the corresponding atmospheric plume. With the aim to recover an atmospheric concentration map of the corresponding atmospheric plume, we study the feasibility and relevance of developing a tomography reconstruction algorithm. The principle is to use multiple laser beam paths in a plane, in order to probe the gas absorption.

Conversely to previous work such as [1], the idea is to reconstruct directly the concentration map from the TDLAS instrument retrieval algorithm, including specific tomographic reconstruction algorithms. However, the well-known algorithms that are used in the biomedical domain cannot be used here because the number of projections is too low. More suitable algorithms have to be developed.

Tomography is an ill-posed problem due to high number of free parameters. A way to reduce the number of these free parameters is to reduce the dimension of the problem. In this work, a neural network architecture, called autoencoder, is used (Figure 1). To train the autoencoder, a dataset of atmospheric concentration plumes was generated using a Gaussian plume model formulation [2] considering that the horizontal and vertical location of the sources is known. Once the autoencoder is trained, the latent space parameters are fitted by minimizing the quadratic error between synthetic spectra and spectra calculated from the maps generated by the decoder. This algorithm will be tested with LES (Large Eddy Simulation) simulations. The laser beam geometry is represented Figure 2. Figure 3 shows the obtained concentration map after optimisation using the absorption spectra.

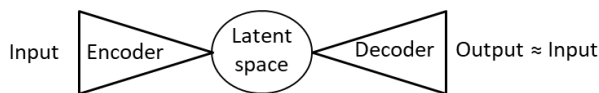


Figure 1 : Autoencodeur principe

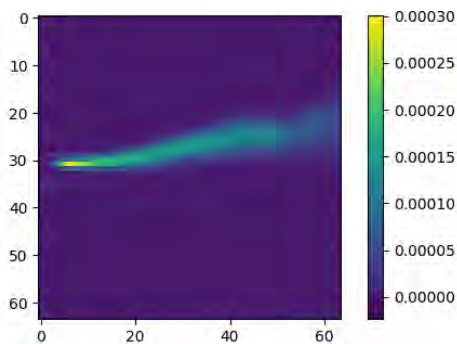


Figure 3 : Obtained concentration map

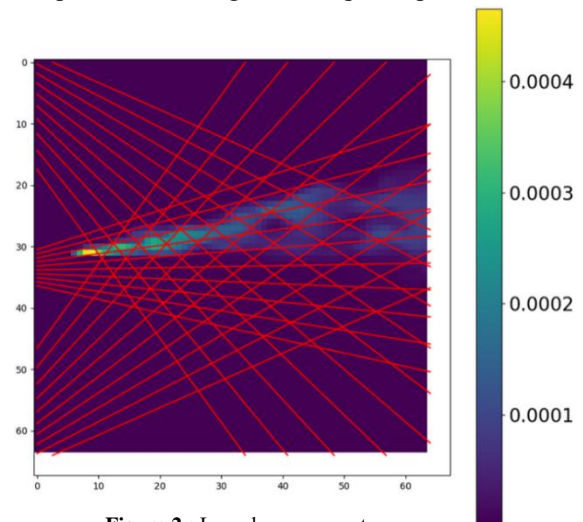


Figure 2 : Laser beam geometry and initial numerically gas plume

## References

- [1] J. Lian *et al.*, « Analysis of temporal and spatial variability of atmospheric CO<sub>2</sub> concentration within Paris from the GreenLITE<sup>TM</sup> laser imaging experiment », *Atmospheric Chem. Phys.*, vol. 19, nov. 2019, doi: 10.5194/acp-19-13809-2019.
- [2] P. Kumar *et al.*, « Mobile atmospheric measurements and local-scale inverse estimation of the location and rates of brief CH<sub>4</sub> and CO<sub>2</sub> releases from point sources », *Atmospheric Meas. Tech.*, vol. 14, sept. 2021, doi: 10.5194/amt-14-5987-2021.

# Design of a low-cost Fabry-Perot cell for Photothermal Spectroscopy

Oscar Bonilla-Manrique<sup>1</sup>, Alejandro Perez<sup>1</sup>, Alejandro Collado<sup>1</sup>, Gabriele Dessena<sup>1\*</sup>

*1. Department of Electronic Technology, Department of Aerospace Engineering, Universidad Carlos III de Madrid, Leganés, 28911, Spain.*

**Short abstract:** The precise detection of NH<sub>3</sub> by Photothermal Spectroscopy is imperative in the development of novel fuels. A compact, low-cost, 3D-manufacturable Fabry-Perot cell is proposed, with thermal control and design optimized for stability, precise alignment and efficient detection in small sample volumes.

In the field of environmental monitoring, gas detection is essential for the continuous control of air quality and the measurement of greenhouse gas (GHG) emissions, especially carbon dioxide (CO<sub>2</sub>). Mitigation strategies for these emissions include the development of carbon-neutral fuels, such as hydrogen and ammonia (NH<sub>3</sub>) [1], with a particular emphasis on "green ammonia," which is produced by electrolysis of water using renewable energy. Infrared optical spectroscopy techniques, such as photothermal spectroscopy (PTS), are effective tools for the accurate and efficient detection of NH<sub>3</sub> is imperative. PTS is based on the absorption of electromagnetic radiation by a gaseous sample, which generates heat that produces a thermal gradient and changes in the refractive index [2]. These changes can be measured by means of a cell with a Fabry-Perot (FP) interferometer. In configurations employing a second laser, this is blocked at a wavelength far from the excitation to avoid interference, synchronizing with the point of maximum sensitivity of the FP cavity. It is imperative that both laser beams intersect with exact precision within the cavity, in the presence of the target gas. The performance of the Fabry-Perot interferometer is contingent on various parameters that affect its efficiency and resolution. Minimal alterations in the curvature of the mirrors can deflect the test beam, thereby affecting the power of the system. This requires meticulous alignment and calibration. Furthermore, thermal variations in the environment and the FP cell have been shown to significantly affect the stability of the system, even with fully stabilized lasers. In light of these challenges, the present work proposes a cost-effective, compact 3D-printable cell design, using metallic materials, to enhance the stability and affordability of the system. As illustrated in fig 1a, the design includes two optical inputs and outputs, facilitating the management of two optical beams (one for excitation and the other for measurement) along two distinct axes. The third axis features a gas inlet and outlet arranged at 60° angles in the upper part. The lower part of the cell is designed to accommodate a Peltier temperature controller, which enables the maintenance of stable cell temperature. This temperature is measured by two thermistors strategically positioned within the cell.

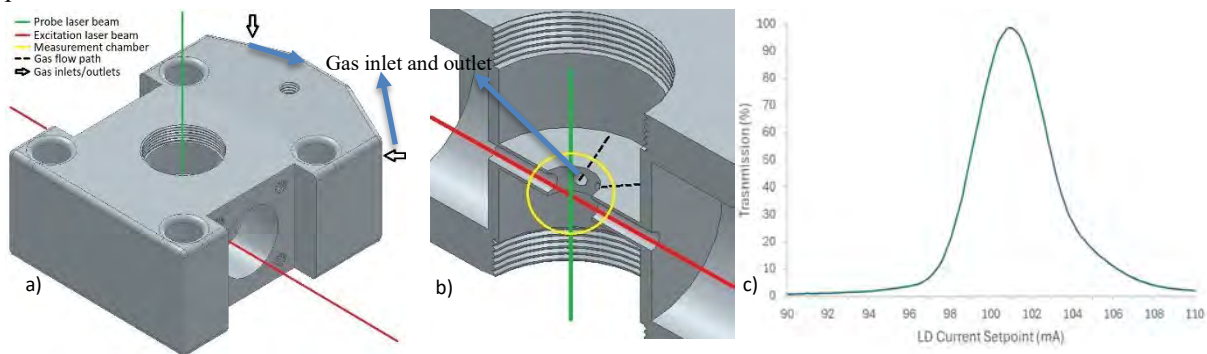


Fig 1. a) Designed FP cell. b) Cavity for the generation of PTS signals. c) FP transmission spectrum.

The cell is designed to use mirrors with a diameter of 12.7 mm and a thickness of approximately 6.35 mm. The laser excitation windows, which are essential for the operation of the device, must have the same diameter and a thickness of approximately 3 mm. The separation between the interferometer mirrors is 2 mm. The gas inlets and outlets are connected to a 1-mm-diameter tube that leads directly to the cavity. The cavity is characterized by a diameter of 4 mm, a height of 2 mm, and four apertures in its walls: two for the inlet and outlet of gas, and two for the inlet and outlet of the excitation laser. This configuration enables the containment of a sample volume of 16  $\mu$ liters. The detailed configuration of this chamber is illustrated in figure Fig 1b. The total dimensions of the cell are approximately 51.4 x 40 x 20 mm. To enhance manufacturing precision, an initial version was created using a 3D printer, and a subsequent version was manufactured using CNC (computer numerical control) machining. This method is cost-effective and allows for tolerances of up to  $\pm 0.02$  mm. The measured spectrum of the manufactured FP cell, as depicted in Fig 1c, substantiates the efficacy of its design.

[1] J. Li et al., "A Review on Combustion Characteristics of Ammonia as a Carbon-Free Fuel," *Front Energy Res*, vol. **9**, (2021).

[2] S. Adhikari, P. Spaeth, A. Kar, M. D. Baaske, S. Khatua, and M. Orrit, "Photothermal microscopy: Imaging the optical absorption of single nanoparticles and single molecules," *ACS Nano*, vol. **14**, no. 12, pp. 16 414–16 445 (2020).



# Development of an Optical pCO<sub>2</sub> Sensor Based on ATR for Deep Sea Applications

Raimund Brunner<sup>1</sup>, Marcel Kamrad<sup>2</sup>, Jochen Erb<sup>1</sup>, Carsten Bolwien<sup>1</sup> and Jürgen Wöllenstein<sup>1,2</sup>

1. Fraunhofer Institute for Physical Measurement Techniques IPM, Georges-Köhler-Allee 301, 79110 Freiburg, Germany

2. Department of Microsystems Engineering – IMTEK, Georges-Köhler-Allee 102, 79110 Freiburg, Germany

3. University of Freiburg, Department of Microsystems Engineering—IMTEK, 79110 Freiburg, Germany

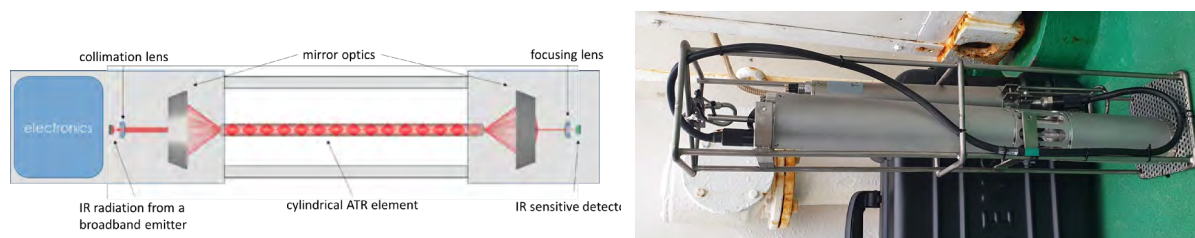
Email: [raimund.brunner@ipm.fraunhofer.de](mailto:raimund.brunner@ipm.fraunhofer.de)

**Short abstract:** This research presents the development of a novel optical pCO<sub>2</sub> sensor using attenuated total reflection (ATR) for deep-sea applications. The membrane-free system operates in the mid-infrared range, achieving response times of seconds and concentration resolution of  $\pm 10$  mg/l at depths up to 200 bar, with ongoing developments focused on sensitivity and drift stability.

As part of the AIMS<sup>3</sup> joint project (CDRmare)[1], a novel optical pCO<sub>2</sub> sensor was developed based on attenuated total reflection (ATR) in the mid-infrared range. The sensor targets real-time monitoring of dissolved CO<sub>2</sub> in saltwater for deep sea applications up to 200 bar.

The measurement principle utilizes the direct interaction of the evanescent field with the medium without membranes, enabling response times in the range of seconds. The optical configuration was optimized through Zemax simulations and consists of a monochromatic ICL-LED ( $\lambda \approx 4.3 \mu\text{m}$ ), a cylindrical ATR element made of sapphire, and a thermoelectrically cooled PVA-3TE-4.5 detector. An axicon mirror geometry was employed for maximum coupling efficiency and optimized absorption path length. A compact electronic design with low-noise amplifier circuitry, LED modulation technology, and an integrated microcontroller enables signal processing and sensor signal evaluation. The sensor achieves a concentration resolution of  $\pm 10$  mg/l with an integration time of 3 seconds in the range of 50–340 mg/l pCO<sub>2</sub>. Calibration is performed using the Henry constant and the CO<sub>2</sub>SYS model.

The pressure-resistant integration was implemented as a cylindrical housing construction made of titanium with a cage structure for the ATR crystal and tested under real field conditions on the research vessel *Littorina*. Current developments focus on optical referencing techniques for temperature drift compensation and extended characterization with variable pressure and salinity parameters.



**Fig. 1** Schematic representation of the sensor concept with optical beam path (left), test probe unit of the pCO<sub>2</sub> sensor for real field measurements in seawater, combined with a P-T sensor (right).

To prepare the attractive ATR sensor concept for broader fields of application, the sensor must be improved in both its detection strength and drift stability. A significant advancement toward a more compact optical design of the pCO<sub>2</sub> sensor will be achieved through the integration of an ICL laser using optical polarization [2]. In the current development phase, a one-sided optical arrangement with reflected beam path is being designed. The source and detection are positioned on the same side of the ATR element; this arrangement not only enables a more compact design but also doubles the effective absorption path length with the same crystal length, potentially improving the sensitivity of the system. In contrast to conventional referencing methods that require a separate spectral reference channel, this approach utilizes the different evanescent polarization properties of the laser light for simultaneous referencing. This method allows significant improvements in compensation of thermal drifts and long-term fluctuations, which is particularly relevant for use under variable environmental conditions in the maritime field.

## References

- [1] Achim Kopf et al., “Initial results of a pilot project for sub-seabed basalt storage of carbon dioxide on the Reykjanes Ridge”, <https://doi.org/10.1016/j.ccst.2024.100265>.
- [2] Stephan Freitag, Matthias Baer, Laura Buntzoll, Georg Ramer, Andreas Schwaighofer, Bernhard Schmauss, and Bernhard Lendl, “Polarimetric Balanced Detection: Background-Free Mid-IR Evanescent Field Laser Spectroscopy for Low-Noise, Long-term Stable Chemical Sensing”, <https://dx.doi.org/10.1021/acssensors.0c01342>, ACS Sens. 2021, 6, 35–42.



# From Design to Device: Efficient Size-Based Separation of Particles in Spiral Microfluidic Chips

Stefania Caragnano<sup>1,3\*</sup>, Isabella Petruzzellis<sup>1</sup>, Angeles Ivon Rodriguez Villarreal<sup>2</sup>, Jasmina Casals Terre<sup>2</sup>, Antonio Ancona<sup>1,3</sup>, Roberto Osellame<sup>4</sup>, Rebeca Martínez Vázquez<sup>4\*</sup>, and Annalisa Volpe<sup>1,3</sup>

1. Physics Department, Università degli Studi di Bari Politecnico di Bari, Via Orabona 4, 70126 Bari, Italy;

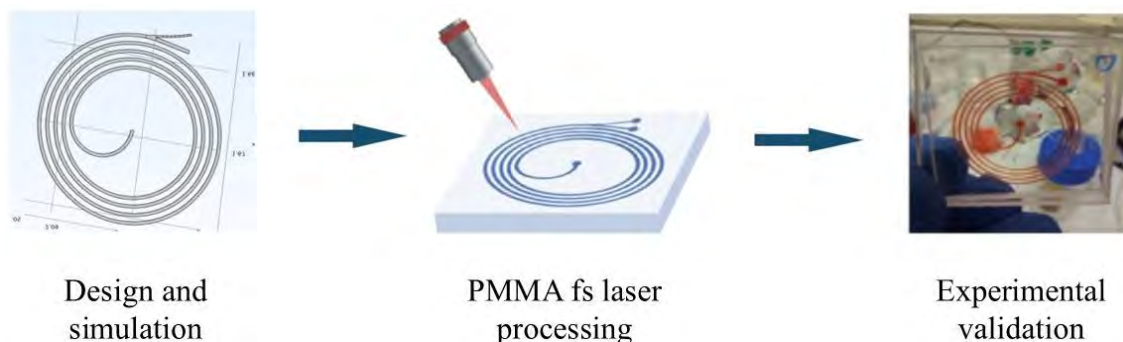
2. Universitat Polytechnica de Catalunya (UPC), 08222 Campus de Terrassa Carrer de Colom I, Spain;

3. Institute for Photonics and Nanotechnologies (IFN), National Research Council, Via Amendola 173, 70125, Bari, Italy;

4. Institute for Photonics and Nanotechnologies (IFN), National Research Council, Piazza L. da Vinci 32, 20133, Milano, Italy;

**Short abstract:** Lab-on-Chip devices have emerged as a revolutionary tool for rare cell extraction. This study unveils an innovative fabrication method that combines simulations, femtosecond laser processing, and experimental validation to create an efficient device for size-based particle separation, marking a significant advancement the field.

The extraction of rare cells, such as circulating tumor cells (CTCs), plays a crucial role in cancer diagnostics and monitoring [1]. Lab-on-Chip (LoC) devices have emerged as a revolutionary tool in this context, enabling the miniaturization of complex laboratory functions onto a single microchip for efficient, real-time particle detection. These devices are widely utilized in diagnostics, biotechnology, and environmental monitoring due to their ability to conduct complex analyses with reduced sample volumes [2]. However, the fabrication of LoC devices requires highly precise and flexible techniques to ensure optimal performance, capable of keeping pace with simulation-driven designs [3]. This study introduces a novel fabrication approach that integrates simulations, femtosecond (fs) laser processing, and experimental validation (see Figure 1) to create a chip designed for inertial size-based particle sorting. Comsol Multiphysics simulations were used to optimize the device design and geometry, enabling precise refining of the microfluidic channels and separation mechanisms. Subsequently, the fs laser was employed to engrave the optimized microfluidic geometry onto a polymethylmethacrylate (PMMA) substrate by varying only the scanning speed parameter, ensuring a highly reproducible, precise, and simple process. This approach successfully produced a microfluidic device with a spiral microchannel design and complex trapezoidal cross-sectional geometry, tailored for the detection and separation of 20  $\mu\text{m}$  diameter particles (simulating circulating tumour cells) from 6  $\mu\text{m}$  diameter particles (resembling red blood cells). Experimental results demonstrated 98.2% separation efficiency for 20  $\mu\text{m}$  particles, in alignment with simulation predictions. The device was further validated using blood samples containing only red blood cells. Combining low-cost materials with a customizable design, this device is well suited for commercialization and for supporting advanced sensing applications in medical diagnostics.



**Fig. 1** Grafical abstract.

## References

- [1] Rapanotti, M. C., Cenci, T., Scioli, M. G., Cugini, E., Anzillotti, S., Savino, L., Coletta, D., Di Raimondo, C., Campione, E., Roselli, M., Bernardini, S., Bianchi, L., De Luca, A., Ferlosio, A., & Orlandi, A. (2024). Circulating Tumor cells: origin, role, current applications, and future perspectives for personalized medicine. *Biomedicines*, 12(9), 2137. <https://doi.org/10.3390/biomedicines12092137>
- [2] Petruzzellis, I., Vázquez, R. M., Caragnano, S., Gaudiuso, C., Osellame, R., Ancona, A., & Volpe, A. (2024). Lab-on-Chip Systems for Cell Sorting: Main features and advantages of inertial focusing in spiral microchannels. *Micromachines*, 15(9), 1135. <https://doi.org/10.3390/mi15091135>
- [3] Pradeep, A., Raveendran, J., & Babu, T. S. (2022). Design, fabrication and assembly of lab-on-a-chip and its uses. *Progress in Molecular Biology and Translational Science*, 121–162. <https://doi.org/10.1016/bs.pmbts.2021.07.021>

# N<sub>2</sub>O Concentration Measurement Based on Multi-Absorption Spectral Signals Analysis Using End-to-End CNN Learning

Gunho Chung<sup>1</sup>, Nakwon Jeong<sup>1,2</sup>, Daehae Kim<sup>1</sup>, Miyeon Yoo<sup>1,\*</sup> and Changyeop Lee<sup>1,\*</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

2. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

**Short abstract:** N<sub>2</sub>O is a potent greenhouse gas, and real-time monitoring is crucial for reducing emissions in display and semiconductor manufacturing. Multi-absorption lines around 8.31  $\mu\text{m}$  are the target of this analysis. It applies convolutional neural network (CNN)-based image analysis to enhance the accuracy of concentration measurements, addressing baseline uncertainties in TDLAS.

Nitrous oxide (N<sub>2</sub>O) is a potent greenhouse gas with a global warming potential approximately that is 300 times greater than carbon dioxide (CO<sub>2</sub>). The semiconductor and display industries, which have been experiencing continuous global expansion, contribute significantly to greenhouse gas emissions, raising environmental concerns. In semiconductor manufacturing, N<sub>2</sub>O is primarily utilized in deposition processes, and the emitted gases are treated using point-of-use (POU) scrubbers. The optimization of scrubber performance necessitates real-time monitoring of N<sub>2</sub>O concentration, for which Tunable Diode Laser Absorption Spectroscopy (TDLAS) serves as a viable and highly sensitive analytical technique [1]. Despite its advantages, TDLAS-based N<sub>2</sub>O quantification is hindered by baseline uncertainty, which can have a significant impact on the reliability of measurement results. Furthermore, the N<sub>2</sub>O absorption spectrum broadens under ambient and high-pressure conditions due to collisional broadening, leading to an expanded spectral wing region [2]. The improper handling of this wing region can adversely affect baseline determination, thereby reducing the reliability of concentration measurements. To mitigate these challenges, a Convolutional Neural Network (CNN)-based image analysis approach was proposed to enhance the accuracy of N<sub>2</sub>O concentration measurements in this study [3]. TDLAS-based detection of N<sub>2</sub>O was conducted under ambient temperature and pressure conditions using a quantum cascade laser emitting at a mid-infrared wavelength of 8.31  $\mu\text{m}$ . The CNN model was trained utilizing a dataset comprising 70% experimental data and 30% simulation data. Experimental validation was performed using a 1-meter optical path length gas cell across a N<sub>2</sub>O concentration range of 0.1% to 10%. The experimental results show that the proposed method can contribute to baseline setting in TDLAS measurements.

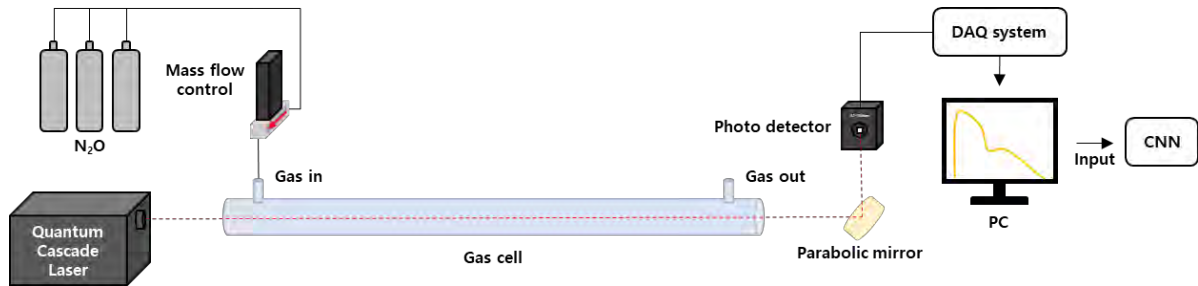


Fig. 1: Schematic experimental setup

## References

- [1] Fengjiao Shen et al., Real-time monitoring of N<sub>2</sub>O production in a catalytic reaction process using mid-infrared quantum cascade laser. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 221, 1-7(2018)
- [2] Christopher S. Goldenstein et al., SpectraPlot.com: Integrated spectroscopic modeling of atomic and molecular gases. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 200, 249–257(2017)
- [3] Yinsong Wang, Shixiong Chen, Qingmei Kong, Jianqiang Gao, Research on CO concentration detection based on deep learning and TDLAS technology, *Optics and Lasers in Engineering*, 181(2024)

# State-of-the-art photoacoustic gas detection adapted to nitric oxide

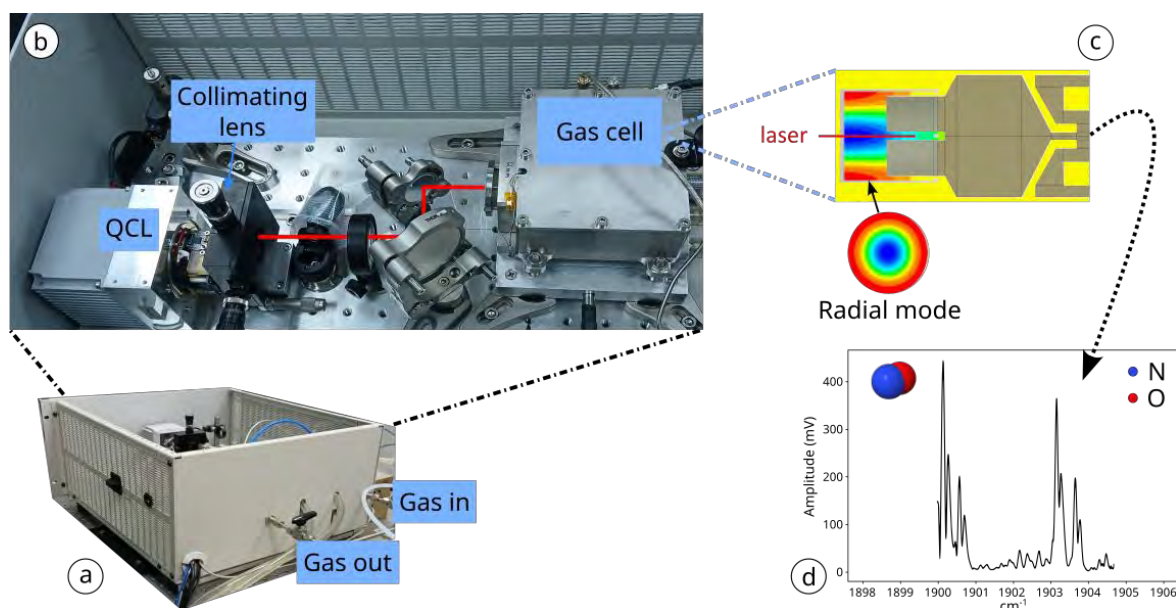
Marie-Hélène Mammez<sup>1</sup>, Maxime Duquesnoy<sup>2</sup>, Jean-Michel Melkonian<sup>2</sup>, Raphaël Levy<sup>2</sup>

1. SATT Paris-Saclay, 86 rue de Paris, 91400, Orsay (France)

2. DPHY, ONERA, Université Paris-Saclay, 6 chemin de la Vauve aux Granges, 91123, Palaiseau (France)

**Short abstract:** We present recent developments on a photoacoustic gas detector employing a custom quartz tuning fork coupled with an acoustic radial resonator. The detector was fully characterized, demonstrating state-of-the-art sensitivity of  $3 \times 10^{-10} \text{ W} \cdot \text{cm}^{-1} \cdot \text{Hz}^{-1/2}$ . Then, it was implemented with a quantum cascade laser into a prototype dedicated to NO measurement in the atmosphere.

Quartz enhanced photoacoustic spectroscopy (QEPAS) is an optical method for trace gas measurements down to a few parts per billion. A QEPAS detector is composed of a quartz tuning fork (QTF) associated to acoustic resonators to enhance the overall sensitivity [1]. Contrary to the traditional “on-beam” configuration, our setup uses an “in-plane” configuration (Fig. 1c) in order to increase the optic-acoustic overlap. A gold mirror was also placed in the back of the acoustic radial resonator to increase the interaction length of the laser beam with the target molecule. Moreover, we used a home-made QTF at  $\sim 21 \text{ kHz}$  optimized for maximum sensitivity at atmospheric pressure [2]. Its coupling with the radial resonator was carefully studied through finite element simulations [3] in order to optimize the sensitivity (Fig. 1c). This coupled resonator was first characterized with a telecom laser diode tuned on the  $6490.05 \text{ cm}^{-1}$  line of  $\text{C}_2\text{H}_2$  before being implemented into a prototype dedicated to NO measurement at  $1900.08 \text{ cm}^{-1}$  with a quantum cascade laser provided by mirSense (Fig. 1a, 1b, 1d).



**Fig. 1** a) Global setup; b) Experimental setup for photoacoustic measurements with a quantum cascade laser; c) In-plane configuration with radial resonator; d) Example of a raw WM spectrum of NO (absolute amplitude).

We will present the impact of the environmental parameters (temperature, pressure) onto the resonators' coupling, the standard deviation, and the limit of sensitivity. In the optimal operation condition, we measured a NNEA of  $3 \times 10^{-10} \text{ W} \cdot \text{cm}^{-1} \cdot \text{Hz}^{-1/2}$ . We have also studied the impact of the gas matrix onto the coupling, particularly the difference between a pure  $\text{N}_2$  matrix and a synthetic air matrix with 20 % of  $\text{O}_2$ . Our photoacoustic detector was implemented to measure NO concentrations in a dry matrix. Despite the vibrational-relaxation of the NO molecule is negatively affected by the absence of  $\text{H}_2\text{O}$ , we have been able to reach a limit of sensitivity ( $1\sigma$ ) of 14 ppb. By adding water vapor to the mix, we obtained an ultimate sensitivity of 3 ppb.

## References

- [1] A.A. Kosterev, Y. A., Bakhirkin, R. F., Curl, F. K. Tittel., “Quartz-enhanced photoacoustic spectroscopy”. *Opt. lett.*, **27**(21), 1902-1904, (2002).
- [2] G. Aoust, R. Levy, B. Verlhac, and O. Le Traon, “Ultra high quality factor resonators operated in fluids”, *Sen. and Act. A: Phys.* **269**, p. 569-573 (2018)
- [3] M. Duquesnoy, J.-M. Melkonian, R.l Levy, G. Aoust, I. Tran, and M. Raybaut, “Photoacoustic gas sensing employing an improved radial resonator”, *CLEO 2023*, May 2023, San Jose, United States. pp.AW3I.6, 10.1364/CLEO\_AT.2023.AW3I.6, hal-04269256

# Partial Least Squares Regression analysis of natural gas-like mixtures using a mid-infrared supercontinuum broadband source

Paola Formica<sup>1</sup>, Andrea Zifarelli<sup>1</sup>, Angelo Sampaolo<sup>1,2</sup>, Hongpeng Wu<sup>2</sup>, Lei Dong<sup>2</sup>, Vincenzo Spagnolo<sup>1,2</sup> and Pietro Patimisco<sup>1,2</sup>

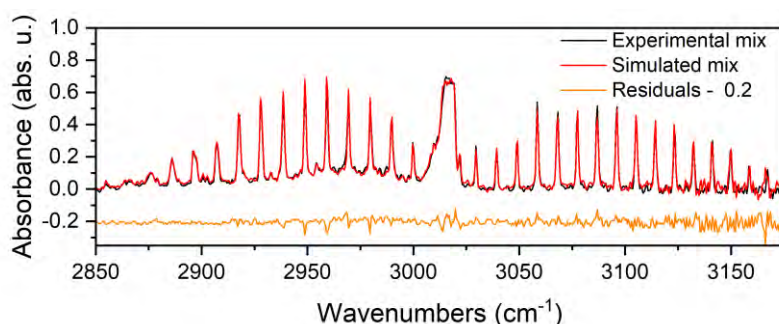
1. Dipartimento Interateneo di Fisica, Polytechnic of Bari & University of Bari, Via G. Amendola 173, Bari 70125, Italy

2. State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Laser Spectroscopy, Shanxi University, Taiyuan, 030006, China

**Short abstract:** We present a broadband mid-infrared gas sensor using direct absorption spectroscopy to reconstruct overlapping absorption bands in natural gas-like mixtures. A comparison between multivariate analysis methods is performed for single-component quantification, showing the superiority of PLSR.

Natural gas (NG) is primarily composed of light hydrocarbons, mainly methane with smaller amounts of ethane, propane, and other trace species. Its composition is monitored to assess calorific value, which reflects its combustibility and, consequently, its quality [1]. Gas chromatography remains the reference technique for this purpose, but it requires multiple detectors, complex setups, and bulky instrumentation, limiting its use in real-time or field monitoring. Optical methods have emerged as fast, non-invasive, and sensitive alternatives. In particular, mid-infrared (MIR) spectroscopy is highly suitable due to strong C-H stretching absorptions in the 3–4  $\mu\text{m}$  range. Unlike narrowband laser-based techniques, which require isolated absorption lines for each species within limited spectral windows, broadband sources enable reconstruction of full absorption bands with overlapping features and unbalanced concentrations. In this context, frequency combs and supercontinuum (SC) sources are the new generation of broadband light sources [2,3]. While dual-comb spectroscopy offers high spectral resolution and sensitivity, its complexity and cost hinder widespread deployment. SC sources, instead, provide a simpler and more cost-effective alternative for simultaneous multi-species gas detection. The spectral information provided by the broadband sources requires advanced data processing. Machine learning-based Multivariate Analysis (MVA), in particular Partial Least Squares Regression (PLSR) represents a solid and reliable approach for spectroscopic analysis for the deconvolution of the spectral contribution of overlapping absorption peaks [4].

In this work, a broadband MIR supercontinuum source was employed to resolve overlapping spectral features in the 2850–3200  $\text{cm}^{-1}$  range. Gas samples, prepared at a 1 :10 dilution to mimic NG mixtures, were passed through an absorption cell and the spectral components of the transmitted light were analyzed using an optical spectrum analyzer with a step resolution of 0.5  $\text{cm}^{-1}$ . For quantitative analysis, the performance of two regression techniques, such as MLR and PLSR, was evaluated on binary and ternary mixtures. The results demonstrated that PLSR outperformed MLR in accuracy. Specifically, MLR yielded mean prediction accuracies of 91% for C1, 68% for C2, and 75% for C3, whereas PLSR achieved 98%, 93%, and 94%, respectively.



**Fig. 1** Comparison between experimental absorbance spectrum of a 7% C1, 0.1% C2 and 0.2% C3 mixture (black) and simulated spectrum reconstructed from a sum of PLSR estimated concentrations (red). Residuals are plotted with a visual shift of -0.2 (orange).

## References

- [1] M. Jaeschke, P. Schley, and R. Janssen-van Rosmalen, "Thermodynamic Research Improves Energy Measurement in Natural Gas," *Int J Thermophys*, vol. 23, no. 4, pp. 1013–1031, 2002, doi: 10.1023/A:1016385902427/METRICS.
- [2] A. Schliesser, N. Picqué, and T. W. Hänsch, "Mid-infrared frequency combs," *Nature Photonics* 2012 6:7, vol. 6, no. 7, pp. 440–449, Jun. 2012, doi: 10.1038/nphoton.2012.142.
- [3] C. R. Petersen *et al.*, "Mid-infrared supercontinuum covering the 1.4–13.3  $\mu\text{m}$  molecular fingerprint region using ultra-high NA chalcogenide step-index fibre," *Nature Photonics* 2014 8:11, vol. 8, no. 11, pp. 830–834, Sep. 2014, doi: 10.1038/nphoton.2014.213.
- [4] A. Zifarelli *et al.*, "Partial Least-Squares Regression as a Tool to Retrieve Gas Concentrations in Mixtures Detected Using Quartz-Enhanced Photoacoustic Spectroscopy," *Anal Chem*, vol. 92, no. 16, pp. 11035–11043, Aug. 2020, doi: 10.1021/ACS.ANALCHEM.0C00075/ASSET/IMAGES/MEDIUM/AC0C00075\_M002.GIF.



# Optomechanics near- to mid-infrared gate based on self-mixing interferometry

Tecla Gabbriellini,<sup>1,2</sup> Chenghong Zhang,<sup>1,2</sup> Francesco Cappelli,<sup>1,2</sup> Iacopo Galli,<sup>1,2</sup>  
Paolo De Natale,<sup>1,2</sup> Andrea Ottomaniello,<sup>3</sup> Alessandro Tredicucci,<sup>4,5</sup> Simone Borri,<sup>1,2</sup> and Paolo Vezio<sup>2</sup>

1. CNR-INO - Istituto Nazionale di Ottica, Largo E. Fermi 6, 50125 Firenze, Italy

2. UniFI and LENS, via N. Carrara 1, 50019 Sesto Fiorentin (FI), Italy

3. Center for Materials Interfaces, Istituto Italiano di Tecnologia, Via R. Piaggio 34, 56025 Pontedera, PI, Italy

4. Dipartimento di Fisica, Università di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy

5. Laboratorio NEST, CNR -- Istituto Nanoscienze, Piazza San Silvestro 12, 56127 Pisa, Italy

**Short abstract:** Affordable, compact, multipurpose, multi-color sensors are emerging as enticing technologies in today's increasingly interconnected world. We propose here a new optomechanics system based on self-mixing interferometry capable of gating together the near-infrared spectral region, which is highly explored for communication, and the mid-infrared one, namely the molecular fingerprint region.

Over the years, self-mixing (SM) interferometry has emerged as a valuable technology for compact sensors as it allows the use of a single device both as a light source and a detector [1,2]. This is particularly useful at longer wavelengths, such as THz and mid-infrared, where the availability of cost-effective room-temperature commercial detectors is limited [3,4]. In SM interferometry, the radiation emitted by a laser is back-reflected by a target and injected directly in the laser waveguide, causing an interference with a phase relation depending on the target position. By monitoring the emitted optical power or the voltage at the laser terminals, it is possible, therefore, to extract information about the target [1-4]. In particular, in this work, the SM signal generated within

a mid-infrared quantum cascade laser (QCL) is used to probe the oscillation of a trampoline membrane induced by near-infrared amplitude-modulated radiation.

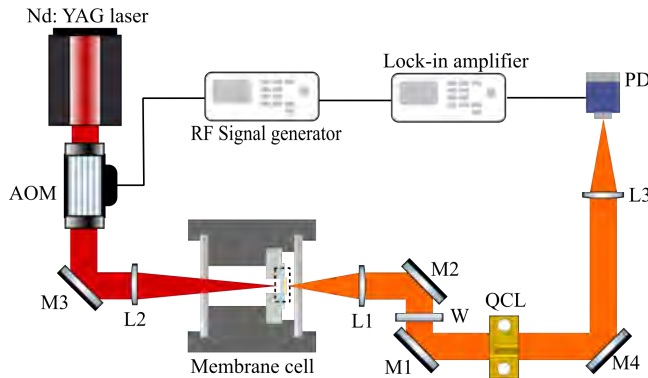


Fig. 1: Setup of the optomechanics system.

A schematic of the assembled setup is depicted in Fig. 1. In detail, the QCL can emit from both the facets, and the front-emitted radiation is used as the probe, while the back-emitted one is used to monitor the SM signal via a photovoltaic detector. The excitation beam is instead obtained by AM-modulating with an acousto-optical modulator

(AOM) the emission of an Nd:YAG laser. In particular, the AOM AM modulation signal is controlled with a lock-in amplifier. Conveniently, the lock-in amplifier takes the SM signal as an input signal and allows to coherently demodulate this signal at the AM modulation frequency. A frequency sweep around the membrane's peak of resonance demonstrates that the AM-modulated excitation beam can induce an oscillation in the membrane via radiation pressure. Furthermore, by demonstrating the QCL's capability to correctly encode the membrane oscillation in the SM signal, we show that the combined optomechanical platform can conveniently operate as a transducer between the two different wavelengths.

## References

- [1] T. Taimre, M. Nikolić, K. Bertling, Y. L. Lim, T. Bosch, and A. D. Rakić, "Laser feedback interferometry: a tutorial on the self-mixing effect for coherent sensing," *Advances in Optics and Photonics* 7, 570–631 (2015).
- [2] L. Columbo, M. Brambilla, M. Dabbicco, and G. Scamarcio, "Self-mixing in multi-transverse mode semiconductor lasers: model and potential application to multi-parametric sensing," *Opt. Express* 20, 6286–6305 (2012).
- [3] S. Hofling, M. Kamp, M. von Edlinger, J. Koeth, and A. D. Rakić, "Demonstration of the self-mixing effect in interband cascade lasers," *Applied Physics Letters* 103, 231107 (2013).
- [4] P. Vezio, A. Ottomaniello, L. Vicarelli, M. Salih, L. Li, E. Linfield, P. Dean, V. Mattoli, A. Pitanti, and A. Tredicucci, "Membrane-mediated conversion of near-infrared amplitude modulation into the self-mixing signal of a terahertz quantum cascade laser," *Photonics* 12 (2025).



# QCL-based ammonia detection: from laboratory to crop field

Csilla Gombi<sup>1</sup>, Anna Szabó<sup>1,2,3</sup>, János Fekete<sup>1,3</sup>, Helga Huszár<sup>1,2,3</sup>, László Horváth<sup>2</sup>, Zoltán Bozóki<sup>1,2,3</sup>

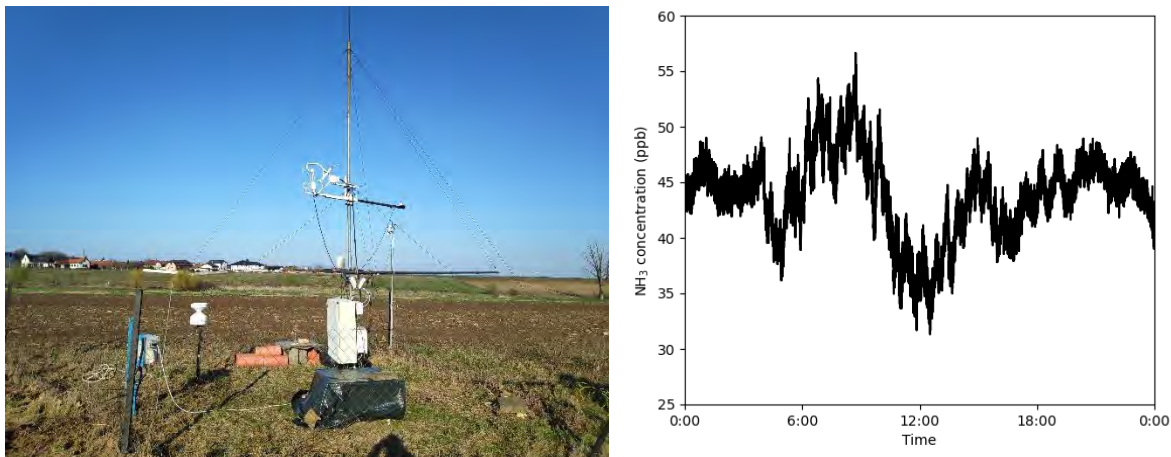
1. Department of Optics and Quantum Electronics, University of Szeged, Szeged, Hungary

2. HUN-REN-SZTE Research Group for Photoacoustic Monitoring of Environmental Processes, Szeged, Hungary

3. Centre of Excellence for Interdisciplinary Research, Development and Innovation of the University of Szeged, 13 Dugonics square, Szeged, 6720, Hungary

**Short abstract:** In this study we present a photoacoustic based system using a 10.3-micron quantum cascade laser to measure ammonia concentrations in agricultural fields. It is designed for long-term field measurements.

From an agricultural and environmental point of view, the measurement of the concentration of atmospheric nitrogen compounds is relevant. Worldwide, less than 50% of applied fertilizers are utilized, while the rest of the nitrogen returns to the environment, causing multiple harmful effects. Measurement of nitrogen loss via the determination of the released gas compounds in situ is a necessary step in reducing emissions. For field measurement of ambient ammonia high sensitivity (ppb level) [1], stability and short response time are required. We have developed a photoacoustic (PA) spectroscopy based system to measure ammonia concentration (and flux) in crop fields, which is capable to continuously measure throughout the entire vegetation period. In our research, we aim to develop a concentration measuring device for long-term field measurements, resistant to weather conditions and external impacts. It is equipped with a continuous-wave 10.3-micron quantum cascade laser (QCL). The system contains a differential, longitudinal PA cell, controlling and data processing electronic units and gas handling. After laboratory assembly and testing, the system was placed in a sunflower field next to a meteorological station (Kartal, Hungary) for an 8-month test measurement. Results of this long-term measurement were consistent with data in literature [2], however, several factors have affected the measurements.



**Fig. 1.** The photoacoustic system and the meteorological station in Kartal (Hungary), and the daily variation of ammonia concentration in June 2024

The main challenge of the QCL based system is that it is highly sensitive to external temperature changes. During the field test, the temperature varied from 5°C to 35°C. Although, the temperature of the PA cell ( $50.00 \pm 0.20^\circ\text{C}$ ) and the QCL ( $20.000 \pm 0.001^\circ\text{C}$ ) were stabilised, it was found that the photoacoustic signal has had a temperature dependence. To address this, we attempted to keep the inside of the instrument box stable at 40°C using an active heating and cooling setup. Additionally, we placed the laser and the sample collection unit on an invar plate, which has the property of minimal thermal expansion. Furthermore, technical amendments have been added to improve the reliability and stability of the system. In March 2025 the system was installed for an other long-term measurement, results of the improved system is discussed.

## References

- [1] K. Wang, P. Kang, Y. LU, X. Zheng, M. Liu, T. J. Lin, K. Butterbach-Bahl, Y. Wang, "An open-path ammonia analyzer for eddy covariance flux measurement." *Agricultural and Forest Meteorology* 308 (2021): 108570.
- [2] M. Insausti, R. Timmis, R. Kinnerely, M. C. Rufino "Advances in sensing ammonia from agricultural sources." *Science of the total environment* 706 (2020): 135124.

**Jeongwoo Ha<sup>1,2</sup>, Jiyeon Park<sup>1,3</sup>, Miyeon Yoo<sup>1</sup>, Daehae Kim<sup>1\*</sup>, Changyeop Lee<sup>1\*</sup>**  
*1. Korea Institute of Industrial Technology (KITECH), 89, Yangdaegiro-gil, Ipjang-myeon, Seobuk-gu, Cheonan-si, Chungcheongnam-do, 31056, KOREA*  
*2. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Repulic of Korea*  
*3. Sungkyunkwan University, 2066, Seobu-ro, 16419, Suwon, Repulic of Korea*

As part of global efforts to reduce greenhouse gas emissions in the industrial sector, conventional fossil fuels are gradually being phased out, and most energy sources are being replaced with carbon-free fuels. In line with this transition, the number of storage facilities for carbon-free fuels is also increasing. Among these fuels, ammonia ( $\text{NH}_3$ ) is classified as a toxic substance. It poses health hazards to humans despite its relatively low explosion risk due to its narrow flammability range and high ignition energy requirement. Therefore, prompt detection is essential in the event of a leak. From the perspective of accuracy, ammonia is a gas that is difficult to measure due to its high reactivity. However, in terms of leak monitoring, the key focus is overcoming spatial limitations. Among quantitative gas analysis methods, sampling-based measurements typically use probes. While this point-based approach provides high accuracy at localized positions, it has limitations in ensuring spatial representativeness in large-area environments. To complement spatial coverage, Tunable Diode Laser Absorption Spectroscopy (TDLAS) can be used. However, this method requires that the laser transmitter and detector be placed at both ends of the gas path, resulting in fixed path configurations and structural constraints depending on the installation environment. To overcome these drawbacks and limitations, this study proposes a method to measure leaked  $\text{NH}_3$  gas concentrations by analyzing backscattering signals using the TDLAS method. The backscattering-based TDLAS technique utilizes the property of molecules to scatter laser light and analyzes the signal composed of the laser reflected backward. Although numerous studies have been reported on methane ( $\text{CH}_4$ ) leak detection using this method, research focusing on  $\text{NH}_3$  remains significantly limited. Thus, this study aims to examine the applicability of this technique to  $\text{NH}_3$  detection [1–2]. Backscattered signals allow the laser transmitter and detector to be installed at the same or nearby locations. This configuration addresses space limitations, and offers increased portability and flexibility, enabling variable measurement paths. Consequently, detecting  $\text{NH}_3$  leaks across broad areas becomes possible while overcoming limitations related to restricted installation space, lack of spatial representativeness, and fixed optical paths. This study employs a near-infrared laser with a center wavelength of  $1.51\text{ }\mu\text{m}$  to detect and analyze the absorption signal of  $\text{NH}_3$  gas for concentration measurements. This technique presents the potential for real-time gas monitoring technology with enhanced spatial representativeness and measurement coverage, especially in pipelines and storage facilities.



[1] Han, Haobin, et al. "All-fiber IPDA lidar for CH<sub>4</sub> leakage monitoring using InGaAs/InP single-photon detector." *Optics Express* 32.21 (2024): 37155-37166.

[2] Diaz, Adrian, et al. "Active standoff detection of CH<sub>4</sub> and N<sub>2</sub>O leaks using hard-target backscattered light using an open-path quantum cascade laser sensor." *Applied Physics B* 122 (2016): 1-11.

# Exploring the Limits of Segmented Circular Multipass Cells

Lorenz Heilmann, Alex Weitnauer, Lukas Emmenegger, Béla Tuzson

*Empa, Laboratory for Air Pollution / Environmental Technologies, Dübendorf, Switzerland*

**Short abstract** Leveraging our Segmented Circular Multipass Cell design, we present a novel fabrication approach enabling cost-effective volume production and compatibility with high-quality coatings and flexible dimensioning, resulting in ultra-compact footprints or optical path lengths up to 1 km.

Segmented Circular Multipass Cells (SC-MPCs) [1] are highly attractive for laser absorption spectroscopy due to their exceptional path-to-volume ratios, straightforward optical alignment, and portability, enabling applications onboard drones or balloons [1,2]. By introducing a new design concept that incorporates additional tilt angles for individual mirror segments, the laser beam can be repeatedly deflected from one supported reflection pattern to another. This allows for multiple uses of the mirror segments, and adjusting the number, position and angular orientation of these segments can dramatically increase the complexity of achievable beam patterns, enabling substantially larger optical path lengths (OPLs) without increasing the cell volume [4].

Leveraging this type of individually tilted SC-MPC, we present a new fabrication technique to further enhance the potential of these cells. Previous cell prototypes were machined into monolithic metal rings, imposing strict constraints on size and mirror quality. As post-polishing is not possible and coating options are limited to metallic coatings, the number of supported reflections is also limited. To address these constraints, we introduced a new fabrication method based on machining mirror segments initially as planar metal strips. These strips can be individually polished and fitted with high-reflectivity dielectric coatings prior to bending them into their final circular shape. This approach allows for high-quality reflective surfaces and greater flexibility in cell design, enabling the fabrication of compact cells (~5 cm diameter) that achieve OPLs exceeding 10 m, as well as larger cells (~50 cm diameter) that support absorption path lengths of 1 km.

We present the method to select among the huge number of possible pattern configurations, along with ray tracing simulations and demonstrate the performance of such SC-MPCs.

## References

- [1] M. Graf, L. Emmenegger and B. Tuzson, "Compact, circular, and optically stable multipass cell for mobile laser absorption spectroscopy," *Opt. Lett.* **43**, 2434–2437 (2018).
- [2] B. Tuzson, M. Graf, J. Ravelid, P. Scheidegger, A. Kupferschmid, H. Looser, R.P. Morales, and L. Emmenegger, "A compact QCL spectrometer for mobile, high-precision methane sensing aboard drones," *Atmos. Meas. Tech.*, **13**(9), 4715–4726 (2020).
- [3] M. Graf, P. Scheidegger, A. Kupferschmid, H. Looser, T. Peter, R. Dirksen, L. Emmenegger, and B. Tuzson, "Compact and lightweight mid-infrared laser spectrometer for balloon-borne water vapor measurements in the UTLS," *Atmos. Meas. Tech.*, **14**(2), 1365–1378 (2021).
- [4] L. Heilmann, M. Graf, A. Weitnauer, L. Emmenegger, and B. Tuzson, "Extending the optical path of segmented circular multipass cells by reiteration of reflection patterns", submitted to *Opt. Lett.* (2025).

# In-situ Diagnostics of Water Vapor and Temperature Distribution Using TDLAS in a Rotating Gliding Arc Plasma Reactor during Dry Reforming of Methane

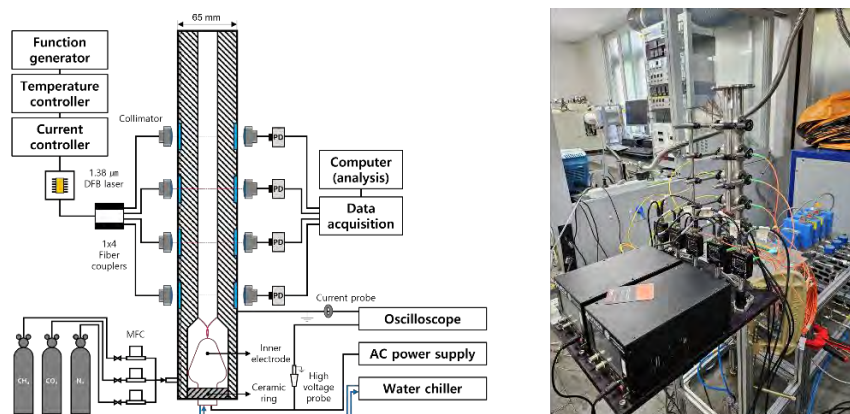
Nakwon Jeong<sup>1,2</sup>, Gunho Chung<sup>1</sup>, Daehae Kim<sup>1</sup>, Miyeon Yoo<sup>1\*</sup>, Changyeop Lee<sup>1\*</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

2. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

**Short abstract:** Real-time, non-intrusive diagnostics of water vapor concentration and temperature distribution in a rotating gliding arc plasma reactor were conducted using tunable diode laser absorption spectroscopy. This enabled quantitative investigation of non-thermal plasma behavior during dry reforming of methane under varying gas compositions, flow rates, and input powers.

Global warming is one of humanity's most pressing environmental challenges, and extensive research is being conducted to convert CO<sub>2</sub>—accounting for approximately 80% of global greenhouse gas emissions—into value-added chemicals or fuels. Among such approaches, dry reforming of methane (DRM), which produces H<sub>2</sub> and CO through the reaction of CO<sub>2</sub> and CH<sub>4</sub>, has garnered significant attention due to its potential to simultaneously utilize two major greenhouse gases, offering both environmental and economic advantages. However, the inherent thermodynamic stability of CO<sub>2</sub> and CH<sub>4</sub> necessitates high temperatures to activate the reaction. Plasma technology enables the generation of highly reactive species such as radicals through electron-impact excitation, ionization, and dissociation processes [1], thereby facilitating CO<sub>2</sub> conversion under milder energy conditions than conventional thermal methods. Among various plasma types, rotating gliding arc (RGA) plasma is classified as a warm plasma within the non-thermal category, exhibiting elevated gas temperatures ranging from 1000 to 3000 K. This characteristic provides a favorable environment for energy-efficient CO<sub>2</sub> decomposition [2]. Water vapor (H<sub>2</sub>O), formed during the DRM process, is a key indicator reflecting the reaction pathways of CO<sub>2</sub> and H<sub>2</sub>. Its concentration and spatial temperature distribution are critical in evaluating reaction characteristics and energy efficiency. Therefore, real-time diagnostics of H<sub>2</sub>O are essential for quantitatively assessing the performance of plasma-assisted DRM processes and elucidating their reaction mechanisms. This study used a rotating gliding arc plasma reactor to measure the concentration and temperature distribution of H<sub>2</sub>O generated during real-time plasma reforming CH<sub>4</sub>, CO<sub>2</sub>, and N<sub>2</sub> mixtures. Tunable diode laser absorption spectroscopy (TDLAS) was employed for this purpose, utilizing the absorption spectrum of H<sub>2</sub>O near 1.38  $\mu\text{m}$ . A butterfly-type DFB laser was used, and the beam was split into four paths aligned along the reactor's axial direction. Each measurement section was spaced 20 mm apart, with an optical path length of 65 mm. The effects of operating parameters on the internal reaction characteristics of the plasma reactor were investigated by quantitatively analyzing the H<sub>2</sub>O distribution and temperature variations under different gas compositions (CH<sub>4</sub>/CO<sub>2</sub>/N<sub>2</sub> ratios), flow rates, and input power conditions. Furthermore, the application of TDLAS demonstrated the feasibility of non-intrusive diagnostics of H<sub>2</sub>O in high-temperature, high-velocity plasma environments, thereby validating its potential for quantitative analysis of non-thermal plasma reactions.



**Fig. 1** Schematic of the experimental setup for in-situ TDLAS diagnostics in a rotating gliding arc plasma reactor.

## References

- [1] M. Ramakers, G. Trenchev, S. Heijkers, W. Wang, and A. Bogaerts, "Gliding arc plasmatron: providing an alternative method for carbon dioxide conversion," *ChemSusChem*. **10**(12), 2642-2652 (2017).
- [2] J. Martin-del-Campo, S. Coulombe, and J. Kopyscinski, "Influence of Operating Parameters on Plasma-Assisted Dry Reforming of Methane in a Rotating Gliding Arc Reactor," *Plasma Chemistry and Plasma Processing*. **40**(4), 857-881 (2020).

# Precision Measurement of OH Radicals in Hydrogen-Blended Flames Using Laser Absorption Spectroscopy

Geunhui Ju<sup>1,2</sup>, Joonmo Son<sup>1</sup>, Miyeon Yoo<sup>1</sup>, Daehae Kim<sup>1\*</sup> and Changyeop Lee<sup>1\*</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

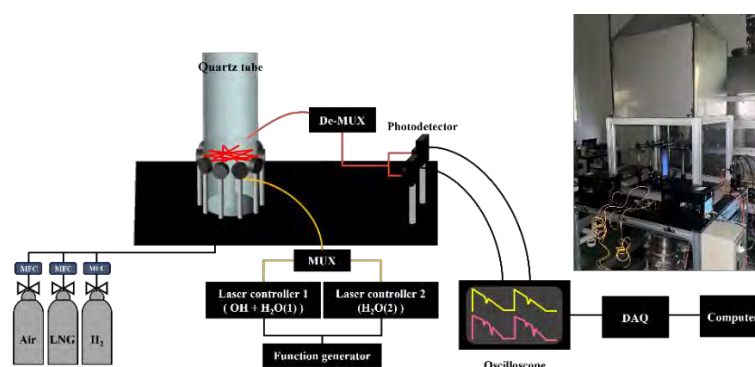
2. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

**Short abstract:** A DAS algorithm was developed for precise OH radical measurement in turbulent combustion. High-resolution data acquisition (4 kHz, 10 MS/s) and wavelet transform-based noise reduction improved signal processing. OH radical concentrations were measured under hydrogen-blended combustion conditions to investigate their variation respect to the hydrogen blending ratio.

Turbulent combustion is highly efficient in generating thermal energy, making it widely applicable in various industrial fields. Understanding the interaction between flame structure, combustion reactions, and turbulent flow is essential for improving combustion efficiency and reducing pollutant emissions[1]. In particular, OH radicals(hydroxyl) play a crucial role in combustion reactions, being vital for flame propagation and chain branching reactions. However, due to high reactivity and short residence time of OH radicals, accurate measurements are challenging, making non-contact spectroscopic techniques a widely used approach for gas species measurement in combustion environments[2-4].

Previous studies have utilized techniques such as chemiluminescence, laser-induced fluorescence(LIF), and laser absorption spectroscopy(LAS). Among these, tunable diode laser absorption spectroscopy(TDLAS) is known for its high sensitivity and real-time quantitative analysis, making it suitable for measuring highly variable radicals in turbulent combustion environments. Typically, in combustion environments where H<sub>2</sub>O is produced, specific wavelengths are selected to measure only the absorption transition of OH radicals. Recently, So et al. proposed an algorithm using direct absorption spectroscopy(DAS) for the simultaneous measurement of temperature, H<sub>2</sub>O, and OH radicals and analyzed the combustion characteristics of flat flames[4]. However, there has been insufficient validation of OH radical measurements using DAS technique in turbulent combustion environments, and the analysis of OH radical signals affected by overlapping H<sub>2</sub>O absorption is needed. In addition, OH radicals exhibit low absorbance in the near-infrared wavelength range, and fluctuations due to turbulence result in highly temporal non-uniform absorption signal intensity.

In this study, we aim to develop the existing DAS analysis algorithm to enhance the precision of OH radical measurements in turbulent combustion environments. To improve the resolution of absorption signals, data acquisition was performed at a sampling rate of 4 kHz and 10 MS/s. Additionally, wavelet transforms were applied for noise reduction and signal processing to enhance concentration analysis. Based on this approach, as shown in Fig. 1, OH radical concentrations were measured according to the hydrogen mixed ratio under hydrogen blended natural gas conditions.



**Fig. 1** Schematic of the experimental setup for OH radical measurement in H<sub>2</sub> blended flame using TDLAS.

## References

- [1] A. Giusti and E. Mastorakos, "Turbulent Combustion Modelling and Experiments: Recent Trends and Developments," *Flow, Turbulent Combust.* **103**(4), 847-869 (2019).
- [2] Y. Liu, J. Tan, M. Wan, L. Zhang, and X. Yao, "Quantitative Measurement of OH\* and CH\* Chemiluminescence in Jet Diffusion Flames," *ACS Omega* **5**(26), 15922-15930 (2020).
- [3] S. Karaminejad, A. E. Moussawi, T. Dreier, T. Endres, and C. Schulz, "Multi-line OH-LIF for gas-phase temperature and concentration imaging in the SpraySyn burner," *Appl. Energy Combust. Sci.* **16**, 100222 (2023).
- [4] S. So, J. Park, M. Yoo, J. Hwang, D. Kim, and C. Lee, "Simultaneous measurement of OH radical, H<sub>2</sub>O concentration, and temperature in a premixed CH<sub>4</sub>/air flame using TDLAS with an improved analysis method," *Opt. Express* **30**(18), 32031-32050 (2022).



# A Study on Measurement of Methane Slip Concentration in Burn-Wet Type POU Scrubber Using TDLAS

Hyungseok Kim<sup>1,2</sup>, Aran Song<sup>1,3</sup>, Daehae Kim<sup>1</sup>, Miyeon Yoo<sup>1\*</sup>, Changyeop Lee<sup>1\*</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

2. Sungkyunkwan University, 2066, Seobu-ro, 16419, Suwon, Republic of Korea

3. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

**Short abstract:** This study measures methane slip in a burn-wet POU scrubber using TDLAS. In semiconductor and display manufacturing, process gases discharged after processing and introduced into the scrubber show high variability in composition and flow rate, causing unburned methane emission due to incomplete combustion. Real time measurement enables optimal combustion control.

Methane slip means that gaseous methane leaks into the atmosphere, occurs in the storage, transportation, and use of LNG with methane as the main component, and during combustion, some of the methane is not oxidized due to incomplete combustion and is exhausted as it is.

Methane slip is being studied mainly in relation to marine ship engines, and exhaust characteristics have been reported [1]. However, in line with the recent greenhouse gas issue, interest in methane slip is also increasing in other fields.

Methane, along with carbon dioxide (CO<sub>2</sub>), nitrous oxide (N<sub>2</sub>O), and fluorinated gases (PFCs, HFCs, SF<sub>6</sub>, and NF<sub>3</sub>), is a major substance that causes global warming. Although methane emissions from the atmosphere are relatively small compared to carbon dioxide, it shows a Global Warming Potential (GWP) that is more than 20 times higher than carbon dioxide based on the same mass, which has a large impact on climate change.

The semiconductor and display industries use POU(point-of-use) scrubbers to reduce emissions of air pollutants and greenhouse gases. Among them, the burn-wet scrubber decomposes the exhaust process gas through high-temperature combustion, and LNG is used as fuel. In this process, methane slip may occur due to the properties of the exhaust process gas or rapid fluctuations in flow rate, and if the methane slip generated from the POU scrubber is reduced, the greenhouse gas reduction effect can be further increased. Therefore, there is a need for a technology that can measure the methane concentration in the exhaust gas in real time and optimally control the scrubber system based on this. However, it is difficult to measure the concentration of certain components in the combustion gas in real time due to the harsh measurement environment at high temperatures. To solve this problem, TDLAS(Tunable Diode Laser Absorption Spectroscopy) technique can be applied. TDLAS is suitable for measuring the concentration of target gas species during combustion in a fast responsive and non-contact manner.

In this study, methane slip characteristics in burn-wet POU scrubber operating conditions in various environments were analyzed through the TDLAS technique, and a TDLAS utilization plan for optimal operation of the scrubber was suggested.

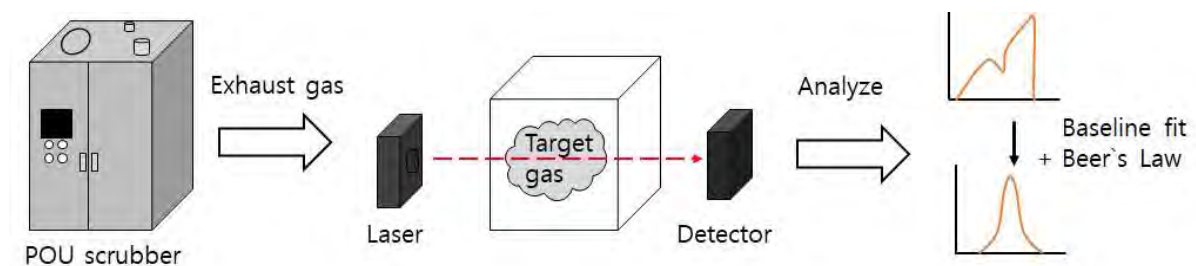


Fig. 1 Experiment set up

## References

[1] Kuittinen, Niina, et al. "Methane slip emissions from LNG vessels-review." *Proceedings of the 30th CIMAC World Congress 2023*.

# Single-board QEPAS system with an open-source FPGA

Luigi Lombardi<sup>1</sup>, Vincenzina Zecchino<sup>3</sup>, Vincenzo Spagnolo<sup>1</sup>, and Cristoforo Marzocca<sup>2</sup>

1. PolySenSe Innovations s.r.l, Via Giovanni Amendola 173, 70126 Bari, Italy;

2. Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, Via Orabona 4, 70125 Bari, Italy;

3. PolySense Lab, Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari 70126, Italy.

**Short abstract:** A compact electronic system for Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) is presented, integrating laser driver, TEC controller, microcontroller and an open-source FPGA on a single board. With low power consumption and high performance, this solution enables portable, high-sensitivity gas sensing, advancing the miniaturization of QEPAS-based detection systems.

This work shows a compact electronic system designed for sensors based on Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS), an advanced technique for trace gas detection. The QEPAS technique combines the high sensitivity of photoacoustic spectroscopy with the unique properties of quartz tuning forks (QTFs), allowing detection limits down to parts per billion. Achieving such sensitivity typically requires precise laser current control and temperature stabilization, which are usually provided by bulky laboratory-grade equipment—limiting the portability and practical deployment of QEPAS systems [1-4]. To overcome these limitations, a highly integrated electronic board was developed, which consolidates all essential functionalities into a compact system. It incorporates a laser driver capable of delivering up to 650 mA with a compliance voltage of 15 V, making it suitable for driving diode lasers, interband cascade lasers (ICLs), and certain quantum cascade lasers (QCLs). It also includes a thermoelectric cooler (TEC) controller with a maximum current of 2.5 A, managed by a digital PID that can be tuned by the user. A microcontroller handles USB-based communication, while an open-source FPGA integrates both the lock-in amplifier and the signal generator, required for laser modulation, as well as all the hardware needed to interface with the preamplifier for signal acquisition and processing.

This single-board enables laser modulation and stabilization, lock-in detection, and control functionalities, significantly reducing system size while improving portability.

Experimental tests demonstrated excellent performance in terms of temperature stability, signal-to-noise ratio and reliability in QEPAS signal acquisition.

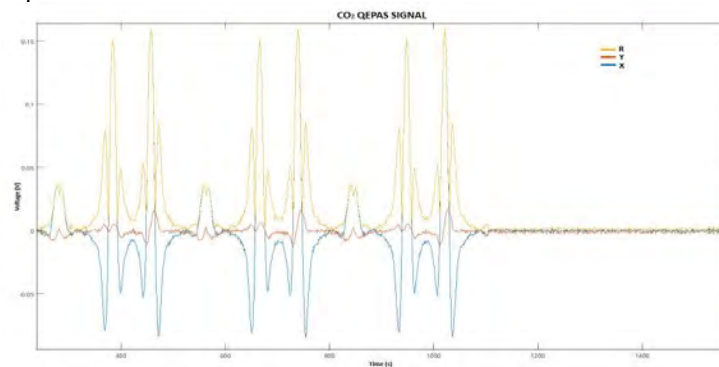


Fig. 1 CO<sub>2</sub> QEPAS signal processed by the board

These results confirm the viability of the compact board as an efficient and low-power solution for QEPAS-based gas sensing, with less than 25 W of maximum power consumption.

By integrating all components into a single PCB, this work represents a substantial progress in the miniaturization of photoacoustic detection systems, paving the way for broader adoption of QEPAS in portable sensing applications.

## References

- [1] A.A. Kosterev, Y.A. Bakhrin, R.F. Curl, F.K. Tittel, "Quartz-enhanced photoacoustic spectroscopy," *Applied Physics B*, vol. 90, no. 2, pp. 165–176 (2008).
- [2] V. Spagnolo, P. Patimisco, F.K. Tittel, "Quartz-enhanced photoacoustic spectroscopy for gas sensing applications," in *Mid-infrared Optoelectronics: Materials, Devices and Applications*, Woodhead Publishing, pp. 597–659 (2020).
- [3] Y. Ma, R. Lewicki, M. Razeghi, F.K. Tittel, "Recent advances in QEPAS-based trace gas sensing," *Applied Sciences*, vol. 8, no. 10, pp. 1822 (2018).

[4] G. Menduni, A. Zifarelli, A. Sampaolo, P. Patimisco, M. Giglio, V. Spagnolo, "Beat Frequency-QEPAS for NO Detection: A Compact Sensor for Environmental Monitoring," *Proceedings of the 2023 PolySense Workshop*, Bari, Italy, May 2023.

# Natural gas detection from an unmanned aerial vehicle (UAV) using remote and photoacoustic sensing based on tunable laser spectroscopy

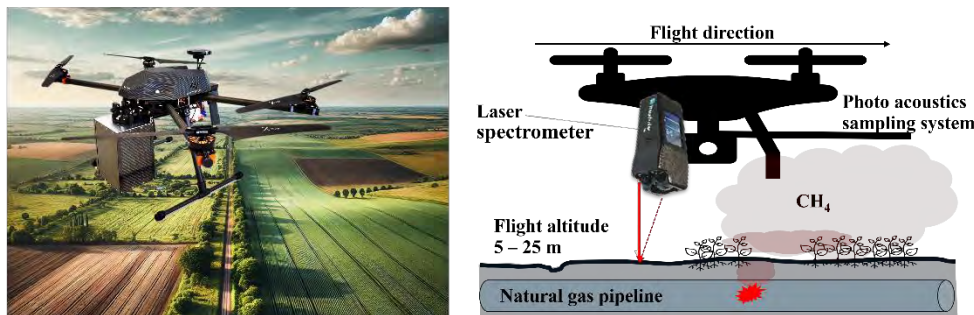
Eric Maier<sup>1,2</sup>, Thomas Strahl<sup>1,2</sup>, Johannes Herbst<sup>1</sup>, Sven Rademacher<sup>1</sup>, Katrin Schmitt<sup>1,2</sup> and Jürgen Wöllenstein<sup>1,2</sup>

1. Fraunhofer Institute for Physical Measurement Techniques IPM, Georges-Köhler-Allee 301, 79110 Freiburg - Germany

2. University of Freiburg, IMTEK, Laboratory for Gas Sensors, Georges-Köhler-Allee 102, 79110 Freiburg - Germany

**Short abstract:** This study discusses the integration of laser-based remote sensing and photoacoustic spectroscopy (PAS) for natural gas detection using unmanned aerial vehicles (UAVs). The system enhances inspection efficiency, achieving high selectivity and sensitivity as well as a measurement rate of 15.25 Hz, thus improving safety and environmental monitoring.

Remote detection of hazardous gases, such as methane – the main component of natural gas – is crucial for various applications, including environmental monitoring and industrial safety [1]. This study introduces an innovative approach to natural gas leak detection using unmanned aerial vehicle (UAV) technology, combining tunable diode laser absorption spectroscopy (TDLAS) for remote methane sensing with an extractive photoacoustic spectroscopy (PAS) device for trace gas detection of methane and ethane. This approach is particularly relevant for inspecting gas infrastructure, as it allows professional operators to deploy laser-based gas measurement devices on UAVs, significantly increasing the efficiency of inspecting gas pipeline networks compared to conventional methods, which involve manually walking along the pipelines with gas detection devices.



**Fig. 1** The system consists of a TDLAS system for remote detection of methane and a PAS system with a gas sampling system including a pump with a flow rate of 300 ml/min for the detection of methane and ethane. The UAV flies at an altitude of up to 25 meters above the ground. The natural gas pipelines are flown over and checked for leaks.

The system distinguishes between natural gas and biogas by measuring methane ( $\text{CH}_4$ ) and ethane ( $\text{C}_2\text{H}_6$ ) concentrations. TDLAS operates in the near-infrared (NIR) at  $1.65\ \mu\text{m}$  for methane detection. Additionally, a PAS system uses an interband cascade laser at  $3.34\ \mu\text{m}$  for methane and ethane measurement in mid-infrared (MIR). Combining backscattering laser spectroscopy and an extractive photoacoustic system (see Figure 1) presents challenges and advantages. TDLAS requires advanced signal processing due to weak backscattered signals but enables calibration-free concentration determination via the HITRAN database. A resolution below  $1\ \text{ppm}\cdot\text{m}$  was demonstrated, and measurements were performed at distances of up to 60 meters with a non-cooperative target. The extractive PAS must efficiently capture gas and minimize downwash effects, offering a detection limit below 20 ppb for  $\text{CH}_4$  and  $\text{C}_2\text{H}_6$ . This is crucial for ethane, which makes up only 0.5–10% of natural gas and helps distinguish it from biogas. Combining PAS and TDLAS ensures reliable leak detection, with TDLAS enabling large-area monitoring in remote detection and the extractive PAS providing maximum sensitivity for small leaks.

The overall system is designed to be lightweight, with a total mass of less than 1 kg, and provides a flight time of up to 30 minutes. The measurement rate of the complete system is 15.25 Hz, yielding a spatial resolution of 0.9 m per measurement point at a flight speed of 50 km/h. This combined technology has the potential to enhance the efficiency of inspections significantly, contributing to improved safety and environmental protection in natural gas infrastructure monitoring.

## References

- [1] R. A. Alvarez et al., "Greater focus needed on methane leakage from natural gas infrastructure," *Proc. Natl. Acad. Sci. USA* **109**, (6435–6440, 2012).
- [2] T. Strahl, M. Bergau, E. Maier, J. Herbst, S. Rademacher, J. Wöllenstein, and K. Schmitt, "Experimental Study to Visualize a Methane Leak of 0.25 mL/min by Direct Absorption Spectroscopy and Mid-Infrared Imaging," *Applied Sciences*, no. **14**, (p. 5988, 2024)

# Reconfiguring the Order of Exceptional Points in a Scalable High-Order Anti-Parity-Time Symmetric System

Xuan Mao, Yu Luo, Qijie Wang

Exceptional points (EPs) are singularities in non-Hermitian systems that feature as two or more eigenvalues and eigenvectors coalesce simultaneously, offering exceptional sensitivity depending on the order of EPs. Especially, in the second-order dissipative coupling system, the eigenvalues exhibit EP shift in the presence of external perturbations or fabrication imperfections. Here, a scalable arbitrary order anti-parity-time (APT) symmetric system is proposed, of which the EPs experience consecutively processes of order decrease, the second-order EP (EP2) shifts, and order increase in response to external perturbations. In a conventional coherent coupling system, EPs are completely disrupted by the perturbation, causing all eigenvalues to deviate from the EPs. On the contrary, when introducing perturbations into the proposed APT system, all eigenvalues divide into one or more pairs, with each pair forming an EP2 indicating that high-order EPs degenerate into one or more EP2s. Counter-intuitively, the order decrease of EPs can also exhibit an enhancement proportional to  $\varepsilon^{1/N}$  upon a perturbation  $\varepsilon$  in an Nth-order system. Notably, one or more EP2s survive in the presence of perturbations, a distinct property making the high-order dissipative system suitable for multiple sensing scenarios in chronological sequences. This property also warrants further exploration of EP-related phenomena under the influence of external perturbations, with the potential to yield significant advancements in the field. These findings will inspire constructing arbitrary order EPs and the design of exceptionally sensitive sensors for real-world applications.



# Comparative study of QEPAS and BF-QEPAS techniques for trace multi-gas detection

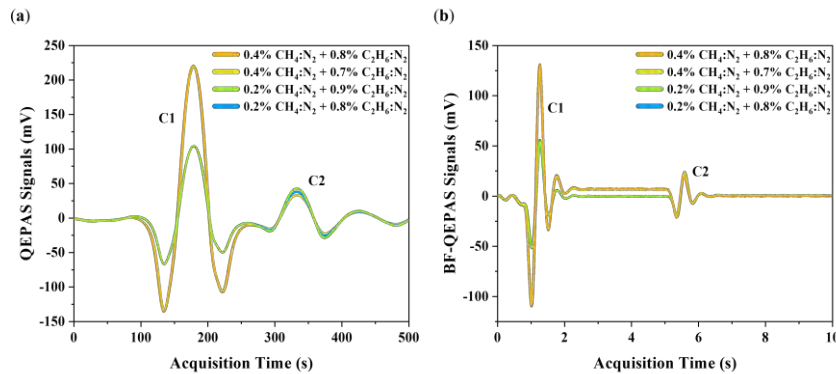
Luigi Melchiorre<sup>1,2</sup>, Giansergio Menduni<sup>1</sup>, Angelo Sampaolo<sup>1</sup>, Giovanni Magno<sup>2</sup>, Vincenzo Spagnolo<sup>1</sup>

1. PolySenSe Lab, Physics Department, Polytechnic University and University of Bari, Via G. Amendola, 173, 70126, Bari – Italy

2. nPEG, Electrical and Information Engineering Department, Polytechnic University of Bari, Via E. Orabona, 4, 70125, Bari – Italy

**Short abstract:** This work compares conventional QEPAS and Beat Frequency QEPAS (BF-QEPAS) for the alternate and sequential detection of methane and ethane. BF-QEPAS significantly reduces measurement time while maintaining comparable sensitivity and eliminating the monitoring of resonator properties, making it ideal for time-sensitive and autonomous gas sensing applications.

We present a comprehensive comparison between Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) and Beat Frequency QEPAS (BF-QEPAS) techniques for the alternate and sequential detection of methane (C1) and ethane (C2) in the near-IR spectral range [1,2]. Although both approaches exploit the same custom-designed Quartz Tuning Fork (QTF) as sensitive element – resonating at 12.3 kHz with a quality factor  $> 8,600$  – coupled with acoustic resonator tubes, they differ fundamentally in signal generation and acquisition methods [3]. The experimental setup incorporates a single optical fiber-pigtailed laser diode emitting at 1,683.53 nm, targeting close absorption features of both C1 and C2. Figures 1a and 1b show both methane and ethane sequential detection employing the QEPAS and BF-QEPAS techniques, respectively.



**Fig. 1** Sequential detection of methane (C1) and ethane (C2) in mixed gas matrices. **(a)** QEPAS signals for various mixtures of CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> diluted in N<sub>2</sub>, acquired during a 500-s scan. **(b)** BF-QEPAS signals for identical gas mixtures obtained in only 10 seconds.

The most significant advantage of BF-QEPAS lies in its dramatically reduced acquisition time. While QEPAS required 500 seconds to complete a full spectral scan capturing both C1 and C2 absorption features, BF-QEPAS requires just 10 seconds for the same type of acquisition. Despite this improvement in measurement speed, BF-QEPAS maintained detection capabilities comparable to conventional QEPAS, achieving 1- $\sigma$  minimum detection limits of 5 ppm for methane and 64 ppm for ethane with an integration time of only 5.097 ms, while QEPAS reached 2 ppm and 20 ppm, respectively, with an integration time as long as 100 ms. Additionally, BF-QEPAS enabled simultaneous determination of gas concentration, QTF resonance frequency ( $f_r$ ) and quality factor ( $Q$ ) from a single measurement. For C1 measurements specifically, this approach retrieved an average  $f_r$  of 12.2 kHz  $\pm$  7 mHz and a  $Q$  of approximately  $9,000 \pm 70$ . This combination of rapid acquisition time, resonance parameters determination, and competitive detection sensitivity establishes BF-QEPAS as an optimal solution for environmental monitoring applications that demand both quick response capabilities and autonomous functioning, particularly in mobile platforms such as unmanned aerial vehicles [4].

## References

- [1] A. A. Kosterev, Yu. A. Bakhtirkin, R. F. Curl, and F. K. Tittel, "Quartz-enhanced photoacoustic spectroscopy," *Opt. Lett.* **27**, 1902 (2002).
- [2] H. Wu *et al.*, "Beat frequency quartz-enhanced photoacoustic spectroscopy for fast and calibration-free continuous trace-gas monitoring," *Nat. Commun.* **8**, 15331 (2017).
- [3] P. Patimisco, A. Sampaolo, M. Giglio, S. Dello Russo, V. Mackowiak, H. Rossmadl, A. Cable, F. K. Tittel, and V. Spagnolo, "Tuning forks with optimized geometries for quartz-enhanced photoacoustic spectroscopy," *Opt. Express* **27**, 1401-1415 (2019).
- [4] A. Sampaolo *et al.*, "Quartz-enhanced photoacoustic spectroscopy for multi-gas detection: A review," *Anal. Chim. Acta* **1202**, 338894 (2022).

# Comparison of an analytical fitting model for direct and indirect spectroscopy techniques

Harald Moser<sup>1</sup>, Johannes P. Waclawek<sup>1</sup> and Bernhard Lendl<sup>1</sup>

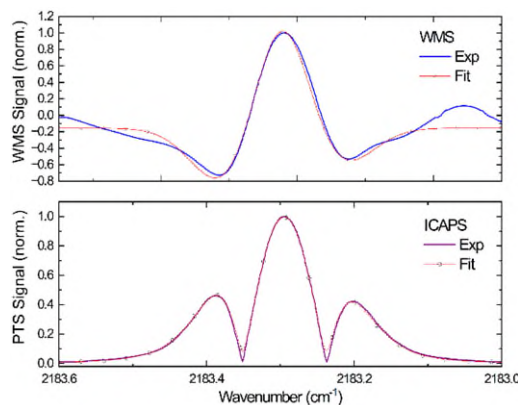
<sup>1</sup>Institute of Chemical Technologies and Analytics, TU Wien, 1060 Vienna, Austria

**Short abstract:** An analytical model for fitting wavelength modulation spectroscopy (WMS) gas spectra acquired by interferometric cavity-assisted photothermal spectroscopy (ICAPS) is presented. The applicability of this model is demonstrated via a comparison of the experimentally recorded data of conventional direct-absorption spectroscopy and ICAPS employing WMS within the same optical setup.

Indirect spectroscopic methods, such as quartz-enhanced photoacoustic spectroscopy (QEPAS) or interferometric cavity-assisted photothermal spectroscopy (ICAPS) may employ 2<sup>nd</sup> harmonic wavelength modulation spectroscopy (2f-WMS) for analyte detection [1], [2]. Here, a suitable spectroscopic excitation light source (e.g. QCL, ICL, LED, etc..) is tuned via a slow saw-tooth profile across the analyte absorption features with simultaneous application of a fast (kHz) sine modulation to the driving current of the excitation source.

The 2f-WMS technique measures a signal roughly proportional to the second derivative of the scanned absorption line shape, hence decreasing the vulnerability to slow baseline drifts and effectively rejecting 1/f noise. In comparison to direct absorption spectroscopy approaches, instrument sensitivity is typically improved by one order of magnitude. Due to the more complex nature of the measured signals, the implementation of simulated and/or measured 2f-WMS reference spectra for derived concentration measurements requires elaborate analytical or numerical simulation of taking crucial parameters of laser wavelength, optical power, modulation depth, absorption line shape, residual amplitude modulation (RAM) of the laser power, and detector response into account. In practice, the majority of 2f-WMS based trace-gas sensors are preferred to be calibrated using reference calibration gas mixtures [3], despite the availability of precise modeling of 2f-WMS spectra [4].

The 7-parameter model is based on a combinational approach of the theoretical works of [4]–[6] with absorbance, peak position, half-width at half-maximum (HWHM), Voigt parameter (d), modulation index (m), linear power modulation amplitude ( $k1v_a$ ) and linear IM/FM phase shift angle ( $\psi$ ). After pre-processing steps of wavelength tuning correction with the aid of reference cells and power normalization with the zeroth or first harmonic (0f, 1f), the experimentally recorded data is non-linear fitted with a constrained Levenberg-Marquardt algorithm implemented in a LabVIEW based program.



**Fig. 1** Fitting results of WMS (top) and ICAPS (bottom) spectra of 100 ppmv carbon monoxide (CO) and with a modulation index of  $m=1.0$ .

## References

- [1] P. Patimisco *et al.*, “A quartz enhanced photo-acoustic gas sensor based on a custom tuning fork and a terahertz quantum cascade laser,” *Analyst*, vol. 139, no. 9, pp. 2079–2087, 2014.
- [2] J. P. Waclawek, H. Moser, and B. Lendl, “Balanced-detection interferometric cavity-assisted photothermal spectroscopy employing an all-fiber-coupled probe laser configuration,” *Opt. Express*, vol. 29, no. 5, p. 7794, 2021.
- [3] P. W. Werle, P. Mazzinghi, F. D’Amato, M. De Rosa, K. Maurer, and F. Slemr, “Signal processing and calibration procedures for in situ diode-laser absorption spectroscopy,” *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.*, vol. 60, no. 8–9, pp. 1685–1705, Jul. 2004.
- [4] P. Kluczynski, J. Gustafsson, Å. M. Lindberg, and O. Axner, “Wavelength modulation absorption spectrometry — an extensive scrutiny of the generation of signals,” *Spectrochim. Acta Part B At. Spectrosc.*, vol. 56, no. 8, pp. 1277–1354, Aug. 2001.
- [5] Y. Liu, J. Lin, G. Huang, Y. Guo, and C. Duan, “Simple empirical analytical approximation to the Voigt profile,” *J. Opt. Soc. Am. B*, vol. 18, no. 5, p. 666, May 2001.
- [6] B. D. Shaw, “Analytical evaluation of the Fourier components of wavelength-modulated Gaussian functions,” *J. Quant. Spectrosc. Radiat. Transf.*, vol. 109, no. 17–18, pp. 2891–2894, 2008.

# Quantitative Analysis of OH Radical Concentration in Turbulent Co-Fired LNG-Hydrogen Flames Using Wavelength Modulation Spectroscopy

Jiyeon Park<sup>1,2</sup>, Jeongwoo Ha<sup>3</sup>, Miyeon Yoo<sup>1</sup>, Daehae Kim<sup>1\*</sup>, Changyeop Lee<sup>1\*</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

2. Sungkyunkwan University, 2066 Seobu-ro, 16419, Suwon, Republic of Korea

3. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

**Short abstract:** Wavelength modulation spectroscopy (WMS) was employed to quantify OH radical concentrations in hydrogen flames. A dual-laser setup with wavelength division multiplexing was used to mitigate H<sub>2</sub>O interference near the 1.49  $\mu\text{m}$  OH absorption line. The normalized 2f signal enabled accurate OH measurements with improved sensitivity and reliability.

With global air quality regulations tightening, the industrial sector is urged to adopt environmentally friendly energy systems. Hydrogen energy, in particular, is emerging as a key alternative for carbon neutrality, prompting efforts to replace fossil fuel-based combustion systems. Developing high-efficiency combustion technology is essential for stable hydrogen use, exhibiting unique combustion characteristics such as high flame speed and strong diffusivity. To control hydrogen combustion stably, assessing the concentration and spatial distribution of OH radicals, key reactive species in flames is essential. OH radicals are important in flame propagation, combustion stability, and reaction mechanism analysis. However, due to their high reactivity and short lifetime, they are rapidly generated and consumed within the flame, making quantitative analysis with sufficient temporal and spatial resolution complex using conventional sampling-based methods. Laser-induced fluorescence (LIF) and chemiluminescence techniques have been employed to address these limitations; however, these methods involve complex setups, high costs, and limited quantitative accuracy. In this study, tunable diode laser absorption spectroscopy (TDLAS), which offers a simple setup and suitability for combustion environments, was used to measure OH radical concentration in hydrogen flames. To extract weak OH signals in trace amounts, wavelength modulation spectroscopy (WMS) was applied to improve the signal-to-noise ratio. [1] A distributed feedback (DFB) laser operating at 1.49  $\mu\text{m}$  in the near-infrared region was used. A 3,000 kcal/hr premixed burner was employed under hydrogen turbulent flame conditions, maintaining an equivalence ratio of 0.98 while varying the hydrogen blending ratio. The spectral region around 1.49  $\mu\text{m}$ , where the central OH absorption line exists, overlaps with the broad H<sub>2</sub>O absorption spectrum in the flame, causing signal interference. To compensate for this, an additional laser at 1.39  $\mu\text{m}$  was introduced, and the optical system was configured using wavelength division multiplexing (WDM) so that both lasers passed through the same spatial and temporal region. Based on two H<sub>2</sub>O absorption signals at 1.39  $\mu\text{m}$ , direct absorption spectroscopy (DAS) was applied to calculate the flame temperature and H<sub>2</sub>O concentration. These values were then used to correct H<sub>2</sub>O interference in the OH analysis. As a result, the peak value of the normalized 2f signal obtained via WMS enabled precise estimation of OH concentration even in the presence of H<sub>2</sub>O interference.

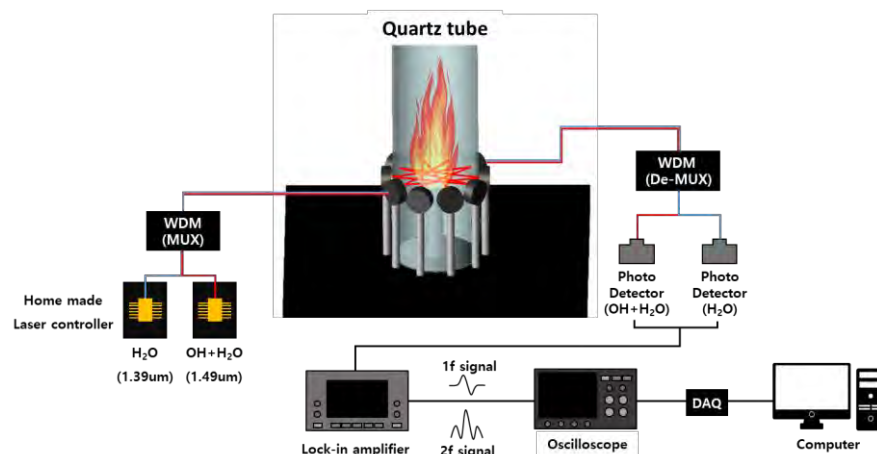


Fig. 1 Schematic of the WMS-based OH Radical Measurement System.

## References

[1] Hayden, T. R., Malarich, N., Petrykowski, D., Nigam, S. P., Christopher, J. D., Lapointe, C., ... & Rieker, G. B. (2019). OH radical measurements in combustion environments using wavelength modulation spectroscopy and dual-frequency comb spectroscopy near 1491 nm. *Applied Physics B*, 125, 1-14.

# Implementation of a CW QCL-based mid-infrared LIDAR

Tecla Gabbriellini<sup>1</sup>, Jacopo Pelini<sup>1</sup>, Lorenzo Mischi<sup>2</sup>, Giovanni Bianchini<sup>1</sup>, Davide Mazzotti<sup>1</sup>, Paolo De Natale<sup>1</sup>, and Simone Borri<sup>1</sup>

<sup>1</sup> CNR-INO and LENS, Via Carrara 1, 50019 Sesto Fiorentino FI, Italy.

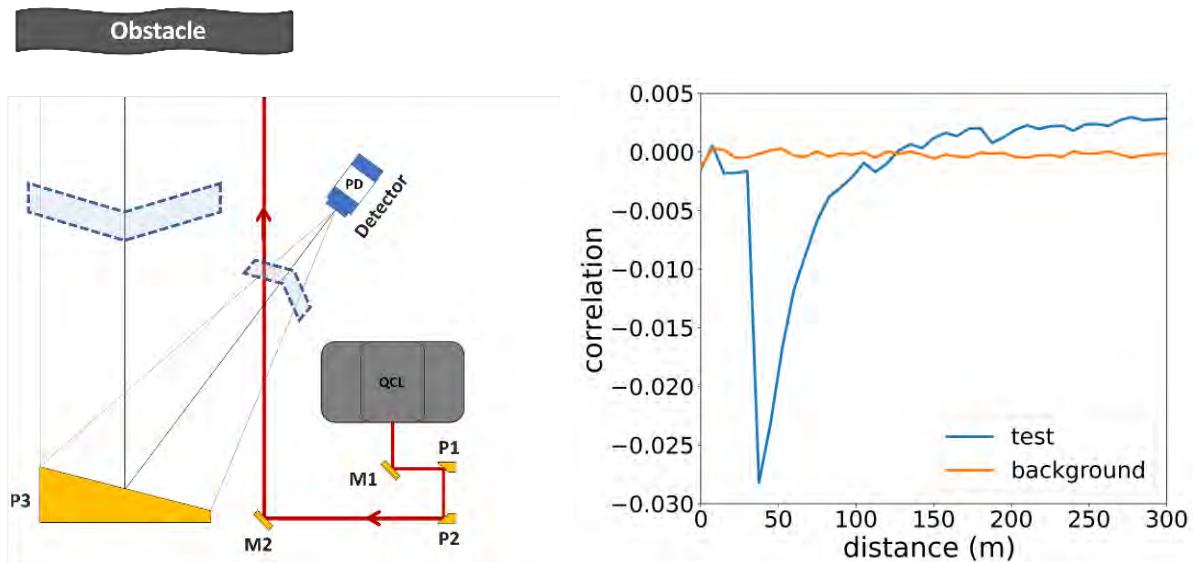
<sup>2</sup> ppqSense S.r.l, Viale L. Ariosto, 492B, 50019 Sesto Fiorentino, FI, Italy

**Short abstract:** Compact and cost-effective remote sensing devices are in high demand in the increasingly interconnected contemporary world. In this framework, we propose a new implementation for Light Detection And Ranging (LIDAR) in the mid-infrared region of the electromagnetic spectrum, using a 4.5 Continuous-Wave Quantum Cascade Laser (CW QCL) and a Pseudo-Random Noise (PRN) modulation technique.

The growing demand for compact and cost-effective systems for remote sensing is motivated by a large number of applications, ranging from remote sensing for atmospheric species like pollutants, aerosol, or particulate matter, to range finding and target identification for safety and security [1]. Driven by the presence of strong absorption lines of several greenhouse/toxic gases (such as CO, CO<sub>2</sub>, N<sub>2</sub>O, O<sub>3</sub>, etc.) combined with low blackbody radiation emission from Sun and Earth, the 4-5  $\mu\text{m}$  band represents an attractive region of the electromagnetic spectrum for addressing efficiently both of these important applications.

Among the pool of optical detection techniques, LIDAR is one of the most used and performing techniques. In LIDAR systems, a high peak power pulsed laser, or a modulated CW source, can be exploited to determine the distance of an object by measuring the time delay between the sent and back-received signals. Furthermore, if the laser is resonant with one absorption feature, it is also possible to perform absorption spectroscopy along the beam path, retrieving information about the specific targeted trace-gas concentration [2,3].

This work aims to combine the potential offered by the LIDAR technology and the advantages given by the mid-infrared transparency window. In our implementation, a PRN technique [4] is exploited to intensity-modulate a CW QCL laser emitting around 4.5  $\mu\text{m}$  with a specific high-frequency digital pattern characterized by null autocorrelation for any non-null shift. The modulated light is guided to a distant target (a scattering obstacle or a reflector), and the back-reflected beam is collected via a detection unit. Thus, the correlation between the detected signal and the modulation pattern will result in a peak at the target distance and (possibly) will retrieve possible absorption features along the optical path. Here, the LIDAR principle and experimental implementation are discussed, together with the characterization measurements and the preliminary outdoor tests.



**Fig. 1** Schematic representation of our mid-infrared PRN LIDAR (left side). An example of correlation measurements using a solid obstacle (i.e. a tree).

## References

- [1] "Lidar - range-resolved optical remote sensing of the atmosphere", vol. 102 of "Springer Series in Optical Sciences", C. Weitkamp ed. (Springer, 2005);
- [2] Quatrevalet, M., et al. "Atmospheric CO<sub>2</sub> Sensing with a Random Modulation Continuous Wave Integrated Path Differential Absorption Lidar." *IEEE J. Sel. Top. Quantum Electron.* 23, 5300311 (2017);
- [3] Lytkine et al., "Range-resolved gas concentration measurements using tunable semiconductor lasers", *Appl. Phys. B* **90**, 339 (2008);
- [4] Takeuchi, N., et al. "Random modulation cw lidar." *Appl. Opt.* 22, 1382 (1983).

# An All-Silicon Metalens operating in the Mid-IR

G. Piscopo<sup>1,2</sup>, A.S. Vorobev<sup>1,3</sup>, J.H. Mendoza-Castro<sup>2,4</sup>, T. Piwonski<sup>3</sup>, G. Magno<sup>2</sup>, L. O'Faolain<sup>1,3</sup>

1. Centre for Advanced Photonics and Process Analysis, Munster Technological University, T12 T66T, Cork, Ireland

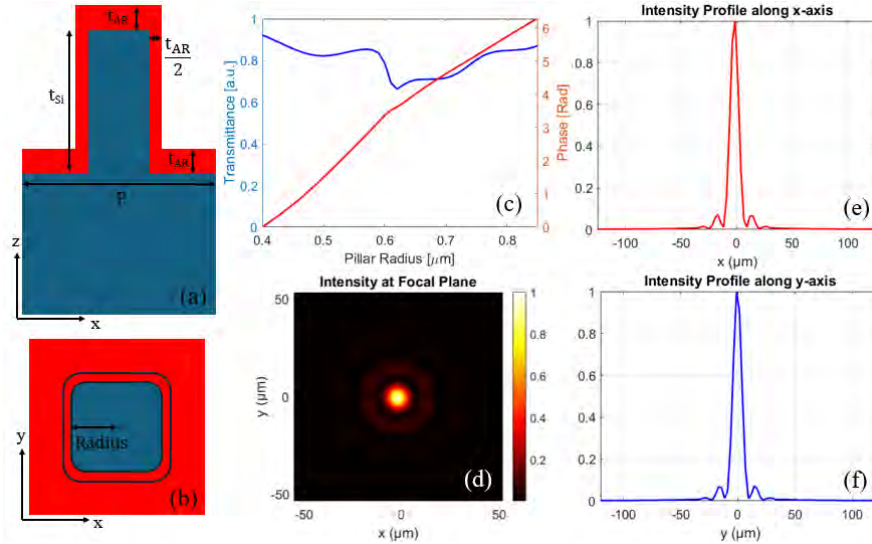
2. Department of Electrical and Information Engineering, Politecnico di Bari, Via E. Orabona, 4, 70126 Bari, Italy

3. Tyndall National Institute, T12 PX46, Cork, Ireland

4. Institute of Chemical Technologies and Analytics, TU Wien, Getreidemarkt 9/164, Vienna, 1060, Austria

**Short abstract:** This work reports the numerical design and characterization of an all-silicon metalens operating at 6  $\mu\text{m}$ . CMOS compatibility and high focusing efficiency render our device a viable candidate as a compact, low-cost, and low-loss Mid-IR free-space optical device.

Metasurfaces are engineered 2D arrays of meta-atoms capable of manipulating light in unique ways. Their applications include amplitude and phase control [1], focusing [2], sensing, spectroscopy [3], and selective mirrors [4]. Among these, especially in the Mid-IR, metasurfaces designed to work as lenses, i.e. metalenses, offer a compact and low-loss alternative to bulky conventional optics.



**Fig. 1** (a) Side view of the unit cell. The parameters are  $P = 2.6 \mu\text{m}$ ,  $t_{AR} = 0.83 \mu\text{m}$ ,  $t_{SI} = 4.5 \mu\text{m}$ . (b) Top view of the unit cell. The pillar radius is swept from  $0.4 \mu\text{m}$  to  $0.85 \mu\text{m}$ , (c) Simulated amplitude and phase as a function of the pillar radius. (d) Normalized spatial intensity distribution in the  $xy$  plane at the focal distance with a 50X magnification on the focal spot. (e)–(f) Normalized intensity profiles at the focal spot along the  $x$  and  $y$  axes respectively.

Figure 1(a)-(b) shows the side and top views of the unit cell, a rounded square silicon pillar on a silicon substrate with a silicon nitride anti-reflection layer. We employed the 3D Rigorous Coupled-Wave Analysis (RCWA) to simulate the amplitude and phase response of the unit cell. By sweeping the pillar radius we obtain a transmitted power above 60% and a full  $0-2\pi$  phase modulation (Figure 1 (c)). The unit cell was then used to design a metalens operating at the central wavelength 6  $\mu\text{m}$  however given the long wavelength a  $\pm 10 \text{ nm}$  working bandwidth is expected. The metalens has a diameter of 5 mm and a focal length of 3.33 mm resulting in a numerical aperture  $NA = 0.6$ . The Huygens-Fresnel principle was employed to extract the normalized spatial intensity distribution in the  $xy$  plane at the focal spot (Figure 1 (d)) and the corresponding intensity profiles at the focal spot along the  $x$  and  $y$  axes respectively (Figure 1 (e)-(f)). From the numerical simulation, we estimated a slight focal spot shift to 3.45 mm and a FWHM at the focal spot of 7.8  $\mu\text{m}$ , slightly larger than the operating wavelength.

**Acknowledgments:** MetaSPECS Project funded by the Science Foundation Ireland (SFI) 21/FFP-A/10002.

## References

- [1] Dagens, B. et al., “Direct Observation of Optical Field Phase Carving in the Vicinity of Plasmonic Metasurfaces,” *Nano Lett.*, Vol. 16, No. 7, 4014–4018, 2016.
- [2] Kotlyar, V. V. et al., “Thin High Numerical Aperture Metalens,” *Opt. Express*, Vol. 25, No. 7, 8158–8167, 2017.
- [3] Mendoza-Castro, J. et al., “Metasurface-Enhanced Mid-Infrared Sensing Based on Integrated Polycrystalline Silicon Metagratings,” *IEEE IHTC*, 1–6, 2024.
- [4] Filograno, F. et al., “Transparent Polymeric Metagrating for Two-Color Reflection in Augmented Reality Displays,” *IEEE IPC*, 1–2, 2024.



# A portable Carbonyl Sulfide laser spectrometer at 4.8 $\mu\text{m}$ for environmental monitoring

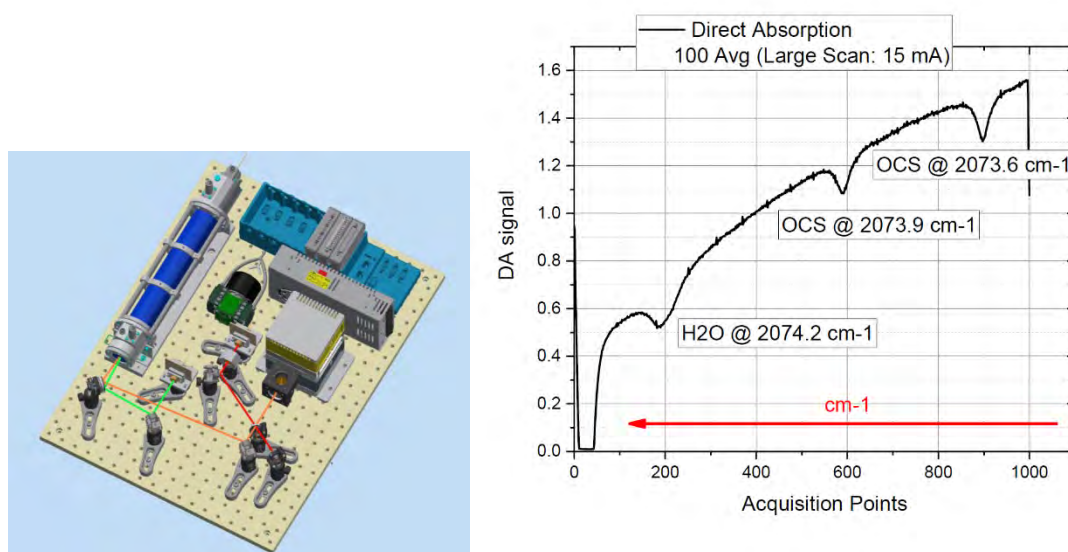
M. Siciliani de Cumis<sup>1</sup>, Stefano Dello Russo<sup>1</sup>, M. Barucci<sup>2</sup>, A. Montori<sup>2</sup>, F. D'Amato<sup>2</sup>, S. Viciani<sup>2</sup>

1. ASI Agenzia Spaziale Italiana - Centro di Geodesia Spaziale, Località Terlecchia, 75100 Matera, Italy

2. CNR-INO - Istituto Nazionale di Ottica, Largo E. Fermi 6, 50125 Firenze, and LENS, via N. Carrara 1, 50019 Sesto Fiorentino, FI, Italy

**Short abstract:** We present a Carbonyl sulfide (OCS) spectrometer based on tunable Quantum Cascade Laser absorption spectroscopy at 4.8  $\mu\text{m}$

Carbonyl sulfide (OCS) is involved in different global cycles: sulphur, carbon and water cycles [1,2,3]. It is present in tropospheric and stratospheric regions. OCS natural sources are volcanos, hot springs, and oceans. OCS also has an important role for biological applications. OCS could be produced in forest or biomass burning. For this reason it is important to monitor it with a portable instrument for field measurements. Here we present a compact prototype for OCS detection. Our instrument is based on a low consumption Quantum Cascade Laser around 4.8 microns provided by Alpes Laser. This laser is also resonant with carbon monoxide and carbon dioxide weak transitions. Due to natural lower OCS concentration, the optical path is enhanced by using a 76-m multipass cell (Aerodyne Research). Electronics is based on compact National Instruments Field Programmable Gate Arrays. This instrument could be easily arranged for both direct absorption and second derivative configuration. The instrument has been validated in both configurations by using an OCS certified mixture.



**Fig. 1** Scheme of the instrument (left). Direct Absorption spectroscopy on OCS certified sample (right)

## References

- [1] Andrea K. Steiger, Yu Zhao, and Michael D. Pluth, ANTIOXIDANTS & REDOX SIGNALING Volume 28, Number 16, 2018 Mary Ann Liebert, Inc. DOI: 10.1089/ars.2017.7119
- [2] Jørgensen BB, Findlay AJ and Pellerin A (2019) The Biogeochemical Sulfur Cycle of Marine Sediments. Microbiol. 10:849. doi: 10.3389/fmicb.2019.00849
- [3] Synthesis to Functional Materials, First Edition. Edited by Xing-Hong Zhang and Patrick Theato. © 2021 WILEY-VCH GmbH.

# TDLAS-Based Tomographic Analysis on OH Radical Distributions in Premixed Flames with irregular Structures

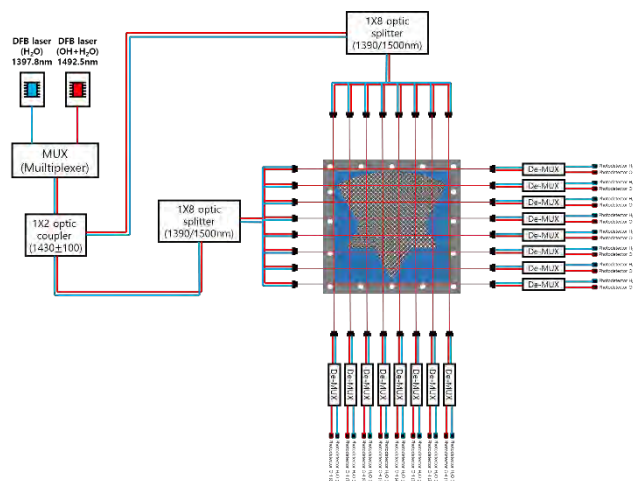
Joonmo Son<sup>1</sup>, Geunhui Ju<sup>1,2</sup>, Miyeon Yoo<sup>1</sup>, Daehae Kim<sup>\*,1</sup>, and Changyeop Lee<sup>\*,1</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

2. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

**Short abstract:** This study uses TDLAS and Tomographic techniques to measure and reconstruct OH radical distributions in premixed methane/air flames, analyzing reconstruction methods to visualize flame dynamics and improve accuracy in reactive flow diagnostics.

The hydroxyl radical (OH) is a representative reactive species generated and consumed during combustion chemical reactions. It serves as a key indicator for visualizing the flame structure and position. The spatial distribution of OH concentration is closely related to the progress of combustion reactions, flame stability, and formation of NO<sub>x</sub>, which is the major precursor for nucleation of ultrafine dust. However, due to OH radicals' high reactivity and short lifetime, accurate concentration measurements require a non-intrusive and real-time diagnostic technique. Tunable Diode Laser Absorption Spectroscopy (TDLAS) is well-suited for this purpose. By applying tomographic reconstruction techniques to the data obtained through TDLAS, it is possible to reconstruct two-dimensional or three-dimensional distributions of gas temperature and concentration over a vast region. In practical combustion systems, flame structures are not stationary; they are subject to continuous variation due to internal turbulence and external flow fields. Therefore, the speed of reconstruction is also important to reflect the transient flame structure. Tomography is a technique that reconstructs spatial distributions of material properties such as velocity, absorptivity, or electrical resistivity. This approach is generally classified into analytical methods and iterative methods. Iterative reconstruction algorithms include ART (Algebraic Reconstruction Technique), MART (Multiplicative ART), SMART (Simultaneous MART), SART (Simultaneous ART), and SIRT (Simultaneous Iterative Reconstruction Technique) [1]. This study employed a combination of TDLAS and tomographic techniques to measure and reconstruct the concentration distribution of OH radicals in premixed methane/air flames with irregular structures. Using five different tomographic algorithms mentioned above, OH concentration distributions were reconstructed from the TDLAS measurements. A quantitative error analysis of the reconstruction results was conducted, and the cause of error were identified to determine the most suitable reconstruction method for each flame condition. Additionally, an ICCD (Intensified Charge-Coupled Device) camera was employed to capture images, allowing comparative analysis between the tomographic reconstruction results and direct optical diagnostics. Experiments were carried out using metal-fiber-based burners with irregular geometries. Based on the acquired data, the distribution of OH radicals was analyzed, and the flames' reactive regions and structural characteristics were visualized.



<Schematic diagram of experiment setup>

## References

[1] Daehae.Kim. A Study on Laser Diagnostics-Based Exhaust Gas Temperature/Concentration Measurement and 2D Image Reconstruction Analysis. PhD diss., Jeonbuk National University Graduate School, 2021. Jeonbuk Special Self-Governing Province.

# Development of Calibration-free Wavelength Modulation Spectroscopy for Precise Measurement of HF, HCl, and NH<sub>3</sub> Emissions in the Semiconductor Industry

Aran Song<sup>1,2</sup>, Hyungseok Kim<sup>1,3</sup>, Daehae Kim<sup>1</sup>, Miyeon Yoo<sup>1\*</sup>, Changyeop Lee<sup>1\*</sup>

1. Korea Institute of Industrial Technology (KITECH), 89 Yangdaegiro-gil, 31056, Cheonan, Republic of Korea

2. Yonsei University, 50 Yonsei-ro, 03722, Seoul, Republic of Korea

3. Sungkyunkwan University, 2066, Seonggyungwan-ro, 16419, Suwon, Republic of Korea

**Short abstract:** This study proposes a calibration-free wavelength modulation spectroscopy (CF-WMS) method for precise measurement of highly reactive gases (HF, HCl, NH<sub>3</sub>) emitted in the semiconductor industry. CF-WMS enables accurate low-concentration gas measurements without periodic calibration, providing a simpler setup than previous methods.

Highly reactive gases, such as HF(hydrogen fluoride), HCl(hydrochloric acid), and NH<sub>3</sub>(ammonia), are used in the semiconductor industry for specific processes: HF and HCl in etching and cleaning and NH<sub>3</sub> in diffusion and deposition. However, the emission of these gases can have severe impacts on both human health and the environment. Specifically, HF and HCl are highly toxic and corrosive, and their release into the atmosphere can lead to acid rain. HF can contribute to global warming by causing ozone layer depletion. NH<sub>3</sub> can cause irritation to the respiratory system, skin, and eyes. In the atmosphere, it undergoes nitrification, converting into nitrate, which is a major component of fine particulate matter (PM<sub>2.5</sub>). This process exacerbates air pollution and deteriorates air quality. For these reasons, many countries strictly regulate the emission levels of HF, HCl, and NH<sub>3</sub>, with the U.S. Environmental Protection Agency (EPA) setting the emission limits to 0.1, 0.1, and 0.2 ppm, respectively. Therefore, accurately measuring and monitoring the concentrations of these gases in semiconductor processes is essential to ensure environmental protection and process safety.

However, as HF, HCl, and NH<sub>3</sub> are highly reactive gases, traditional sampling methods suffer from issues such as gas adsorption and chemical reactions, which interfere with accurate concentration measurement. TDLAS enables non-contact line-averaged measurements, making it an ideal technology for emission monitoring and optimizing emission control systems in semiconductor facilities. This method employs high-resolution spectroscopic techniques to measure gas concentrations in real-time, enabling accurate measurements even for highly reactive gases.

Among the TDLAS techniques, Wavelength Modulation Spectroscopy (WMS) is particularly suitable for measuring gas concentrations below 0.1 ppm, as required by emission limits. However, WMS requires periodic calibration, and the calibration procedure is complex and time-consuming. To resolve this issue, this study adopts Calibration-free Wavelength Modulation Spectroscopy (CF-WMS). Building on the work of Sun [1], this study develops a simplified CF-WMS approach that enables accurate gas concentration measurements without the need for calibration.

In this study, CF-WMS was applied using a 1-meter static cell with 2.3  $\mu\text{m}$  ICL, 3.6  $\mu\text{m}$  ICL, and 9.5  $\mu\text{m}$  QCL to measure the concentrations of HF, HCl, and NH<sub>3</sub> gases, with reference gases used to verify the accuracy and reliability of the experimental results.

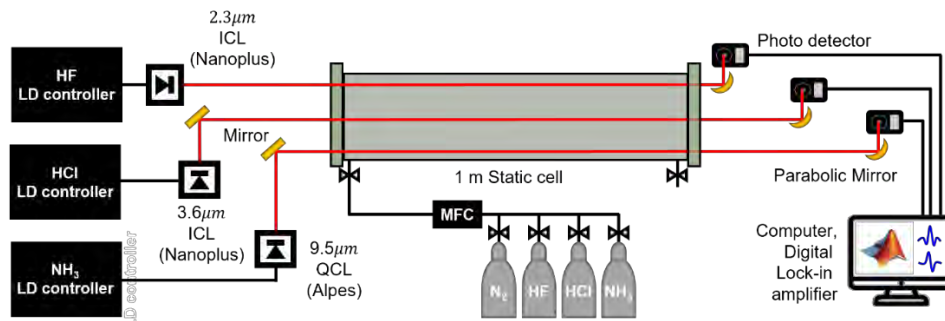


Fig. 1 Schematic of the experimental setup.

## References

[1] Sun, K., Chao, X., Sur, R., Goldenstein, C. S., Jeffries, J. B., & Hanson, R. K., "Analysis of calibration-free wavelength-scanned wavelength modulation spectroscopy for practical gas sensing using tunable diode lasers", *Meas. Sci. Technol.*, **24**(12) 125203 (2013).

# GC-MS-Based Breath Analysis for Early Detection of Colorectal Cancer: A Non-Invasive Diagnostic Approach

Silvano Spagnolo<sup>1,2</sup>, Nicoletta Ardito<sup>1</sup>, Arianna Elefante<sup>1,3</sup>, Marilena Giglio<sup>1</sup>, Arcangelo Picciariello<sup>4</sup>, Leonardo Vincenti<sup>5</sup>, Agnese Dezi<sup>5</sup>, Angelo Sampaolo<sup>1,2</sup>, Alessia Di Gilio<sup>6</sup>, Jolanda Palmisani<sup>6</sup>, Gianluigi De Gennaro<sup>6</sup>, Vincenzo Spagnolo<sup>1,2</sup>

1. PolySense Lab, Dipartimento Interateneo di Fisica, University and Polytechnic of Bari, Via Amendola 173, 70126 Bari, Italy

2. PolySense Innovations srl, Via Amendola 173, 70126 Bari, Italy

3. CNR-INF Udr. Bari, Via Amendola 173, 70126 Bari, Italy

4. Department of Experimental Medicine, University of Salento, 73100 Lecce, Italy

5. Surgical Unit, IRCCS de Bellis, Castellana Grotte, Bari, Italy

6. Department of Biosciences, Biotechnologies and Environment, University of Bari Aldo Moro, Via Orabona 4, 70126 Bari, Italy

## Short abstract:

Colorectal cancer (CRC) remains a leading cause of cancer-related mortality worldwide. Although current screening methods, such as the fecal immunochemical test, have enhanced early detection rates, they are limited by reduced sensitivity for advanced adenomas and a high incidence of false positives. Breath analysis has emerged as a promising non-invasive approach for disease detection and monitoring, including cancer.

In this study, we employed gas chromatography–mass spectrometry (GC-MS) to profile volatile organic compounds (VOCs) in the exhaled breath of CRC patients. Breath samples were collected using the Mistral breath sampler (Fig. 1) following standardized protocols, and VOCs were analyzed to identify metabolic signatures associated with colorectal tumorigenesis. Distinct VOC profiles—particularly involving short-chain alkanes, aldehydes, and aromatic compounds—were observed in CRC patients compared to healthy controls. Notably, compounds such as pentane, hexanal, and benzene derivatives were identified as potential biomarkers reflecting oxidative stress and altered lipid metabolism.

The analytical method demonstrated high reproducibility and sensitivity, capturing subtle metabolic alterations characteristic of malignancy. These preliminary findings support the clinical utility of GC-MS-based breath analysis as a rapid, reliable, and non-invasive tool for early CRC diagnosis, warranting further validation in large-scale studies.



**Fig. 1** Mistral Breath sampler employed for the collection of exhaled breaths.

## References

- [1] A. Picciariello, A. Dezi, L. Vincenti, M.G. Spampinato, W. Zang, P. Riahi, J. Scott, R. Sharma, X. Fan, D.F. Altomare, “Colorectal Cancer Diagnosis through Breath Test Using a Portable Breath Analyzer—Preliminary Data,” *Sensors* **24**, 2343 (2024).
- [2] A.M. Aresta, N. De Vietro, A. Picciariello, M.T. Rotelli, D.F. Altomare, A. Dezi, G. Martines, A. Di Gilio, J. Palmisani, G. De Gennaro, , C. Zambonin, “Volatile Organic Compounds Determination from Intestinal Polyps and in Exhaled Breath by Gas Chromatography–Mass Spectrometry”, *Applied Sciences* **13**, 6083 (2023).
- [3] Arcangelo Picciariello, Donato F. Altomare, *Volatile Organic Compounds: New Potential Biomarkers for Colorectal Cancer*, Springer Cham, Switzerland (2025).

# ATR-FTIR Spectroscopy of Blood Serum for Early, Non-Invasive Detection of Gastrointestinal Cancers

Daphne Spagnolo<sup>1,2</sup>, Andrea Zifarelli<sup>1</sup>, Vitoantonio Bevilacqua<sup>3</sup>, Antonio Brunetti<sup>3</sup>, Arcangelo Picciariello<sup>4</sup>, Agnese Dezi<sup>5</sup>, Leonardo Vincenti<sup>5</sup>, Vincenzo Spagnolo<sup>1,2</sup>

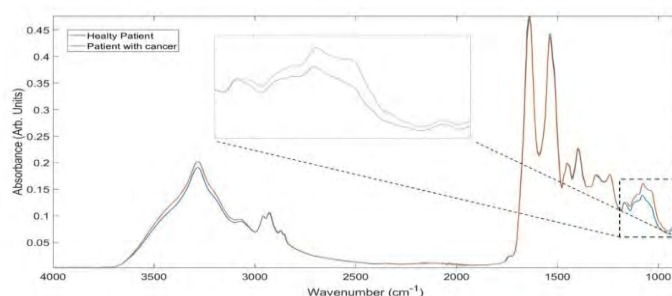
1. PolySense Lab, Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari, 70126 Italy
2. PolySense Innovations srl, Via Amendola 173, Bari, 70126 Italy
3. Department of Electrical and Information Engineering - Politecnico of Bari, Via Orabona, 4, 70125, Bari – Italy
4. Department of Experimental Medicine, University of Salento, 73100 Lecce, Italy;
5. Surgical Unit, IRCCS de Bellis, Castellana Grotte, Bari, Italy

**Short abstract:** We report on a study aiming to demonstrate the potential of ATR spectroscopy combined with machine learning to analyze blood serum for early, non-invasive detection of GI cancers, offering a promising screening method to distinguish healthy individuals from affected patients.

The early detection of gastrointestinal (GI) cancer requires fast, reliable, and minimally invasive diagnostic method, an area where optical absorption spectroscopy holds significant promise. Recently, Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectroscopy has been explored as a tool for identification of different pathologies by means of biofluids analysis (liquid biopsy) [1-3]. Benefitting from minimal sample preparation and reduced sample volume ( $\sim\mu\text{L}$ ), this approach represents a solid candidate for diagnostic application. However, its use in clinical routine is still limited by: fragmented data, lack of medical interpretation, empirical approaches and data analysis complexity. Therefore, this study aims to establish a standardized acquisition protocol using ATR-FTIR spectroscopy to analyse blood serum spectra from both healthy individuals and patients diagnosed with various GI cancers.

Following a pre-analytical optimization, absorption spectra from healthy controls and patients samples were collected in the mid-IR spectral range. Then, the collected spectral data were compared revealing subtle yet meaningful differences between the two groups, as shown in Fig. 1. These differences were further refined through feature selection, and the most diagnostically relevant features were then used to train classification algorithms designed to perform binary classification (e.g., PLS-DA, SVM, etc.), to effectively distinguish among healthy samples and GI cancer.

By enabling accurate analysis based on a simple, minimal, blood sample, this approach contributes to the development of non-invasive screening tools capable of identifying GI cancers at early, often asymptomatic stages, potentially improving patient outcomes through earlier intervention.



**Fig. 1** Comparison between blood serum ATR spectra of a healthy patient and a patient with GI cancer.

## References

- [1] S. Guo, G. Wei, W. Chen, C. Lei, C. Xu, Y. Guan, T. Ji, F. Wang, H. Liu. "Fast and Deep Diagnosis Using Blood-Based ATR-FTIR Spectroscopy for Digestive Tract Cancers," *Biomolecules* **12**, 1815 (2022).
- [2] C. Hughes, M. Brown, G. Clemens, et al. "Assessing the challenges of Fourier transform infrared spectroscopic analysis of blood serum," *J Biophotonics* **7**, 180-188 (2014).
- [3] N. Pang, W. Yang, G. Yang, et al. "The utilization of blood serum ATR-FTIR spectroscopy for the identification of gastric cancer," *Discov Onc* **15**, 350 (2024).



# Advanced Spectroscopic Approaches for Trace Gas Detection in Challenging Matrices

Bo Sun<sup>1,2</sup>, Lijun Qiao<sup>1,2</sup>, Mingjiang Zhang<sup>1,2</sup>, Liantuan Xiao<sup>1,2</sup>

1. College of Physics and Optoelectronics, Taiyuan University of Technology, Taiyuan 030024, China

2. State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Laser Spectroscopy, Shanxi University, Taiyuan 030006, China

**Short abstract:** Accurate trace gas detection in complex environments remains a critical challenge due to matrix interference and ultra-low concentrations. QEPAS leverages quartz tuning forks for high-sensitivity acoustic detection, while LITES employs photothermal effects for non-contact measurement, together enabling effective trace gas analysis in fields such as electrical equipment monitoring and environmental safety.

Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) and Light-Induced Thermoelastic Spectroscopy (LITES) have emerged as powerful techniques for highly sensitive gas detection [1]. QEPAS employs quartz tuning forks (QTFs) as acoustic transducers, leveraging their inherent resistance to environmental noise for high-sensitivity trace gas detection [2]. LITES utilizes QTFs as photothermal detectors, measuring gas concentration through light absorption-induced thermal effects [3]. This circumvents limitations of conventional photoacoustic cells and photodetectors, offering new avenues for gas analysis in complex environments. Their high sensitivity, compact size, and cost-effectiveness render them promising tools for gas detection in challenging matrices.

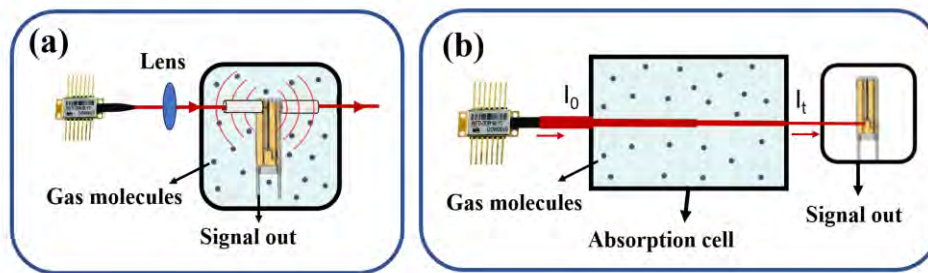


Fig. 1. Schematic diagrams of (a) QEPAS and (b) LITES for trace gas detection.

Our work highlights innovative contributions to spectroscopic gas sensing through advancements in QEPAS and LITES, enabling precise trace gas detection in complex environments. To address the urgent need for gas sensors in early fault diagnosis for SF<sub>6</sub>-insulated electrical equipment, we conducted the following research: For SF<sub>6</sub> decomposition product CO detection, we developed a QEPAS sensor based on a customized T-grooved quartz tuning fork, leveraging its high-quality factor in SF<sub>6</sub> matrices to overcome interference and achieve ppb-level detection, critical for GIS safety. For SF<sub>6</sub> decomposition product H<sub>2</sub>S detection, we developed a LITES-based sensor that integrates a mini-multipass cell, utilizing the non-contact advantage of LITES to enable rapid, ppb-level detection in SF<sub>6</sub> matrices for GIS condition assessment. To address broader gas sensing challenges in complex environments, we proposed Optical Synchronous Signal Demodulation (OSSD) based QEPAS, successfully applied to remote, multi-point methane detection. This overcame traditional QEPAS distance limitations, validated in campus sewer environments, showcasing OSSD-QEPAS for environmental safety monitoring. Furthermore, to broaden the application scope of spectroscopic sensing, we integrated long-wavelength infrared quantum cascade lasers (QCLs) with QEPAS, creating a highly selective and sensitive detection system for VOCs like benzene, toluene, and propane. This system leverages the low spectral cross-interference of the 13-15 $\mu$ m infrared range in VOC detection, significantly improving VOC detection accuracy in complex matrices.

## References

- [1] Y. Ma, "Recent advances in QEPAS and QEPTS based trace gas sensing: a review" *Front. Phys.* **8**, 268 (2020).
- [2] J. Wang, H. Wu, A. Sampaolo, P. Patimisco, V. Spagnolo, S. Jia, L. Dong, "Quartz-enhanced multiheterodyne resonant photoacoustic spectroscopy" *Light Sci. Appl.* **13**, 77 (2024).
- [3] T. Wei, A. Zifarelli, S. Dello Russo, H. Wu, G. Menduni, P. Patimisco, A. Sampaolo, V. Spagnolo, L. Dong, "High and flat spectral responsivity of quartz tuning fork used as infrared photodetector in tunable diode laser spectroscopy" *Appl. Phys. Rev.* **8**, 041409 (2021).

# Photoacoustic instruments for the detection and localization of leaks in refrigeration systems

Panna Végh<sup>1,4</sup>, Bence Molnár<sup>4</sup>, Piroska Ailer<sup>4</sup>, Zoltán Bozóki<sup>1,2,3,4</sup>, Helga Huszár<sup>3,4</sup>

*1 Department of Optics and Quantum Electronics, University of Szeged, 9 Dóm Square, Szeged, 6720, Hungary*

*2 Hilase Development, Production, Service and Trading Ltd., 72-100. Berényi út, Székesfehérvár, 8000, Hungary*

*3 HUN-REN-SZTE Research Group for Photoacoustic Monitoring of Environmental Processes, 9 Dóm Square, Szeged, 6720, Hungary*

*4 Centre of Excellence for Interdisciplinary Research, Development and Innovation of the University of Szeged, 13 Dugonics square, Szeged, 6720, Hungary*

**Short abstract:** The need for reliable and sensitive leak detection has become increasingly critical due to regulatory bans on refrigerants with a high global warming potential. A potential option is a highly sensitive photoacoustic instrument for accurate, fast, and easy leak detection, as demonstrated by our simulation and measurement results.

Refrigerant leaks are a common problem that can significantly affect the efficiency of refrigeration systems and the environment. In particular, the emission of hydrofluorocarbon refrigerants (HFCs) is increasing, mainly because they are widely used as a replacement for chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs), since the Montreal Protocol was agreed [1,2]. Despite their many benefits, HFCs are potent greenhouse gases. Their use is strictly limited, as the current European F-gas regulation establishes restrictions on the use of fluoride refrigerants with a high global warming potential (GWP). The prohibition of high GWP refrigerants has increased the demand for accurate devices to measure fugitive emission losses. According to the F-gas regulations (Regulation (EU) No. 573/2024), a leak detector must have a sensitivity of 5 g/year.

This study aimed to develop a high-precision detection system capable of measuring refrigerant concentrations at the ppm level. The photoacoustic (PA) instrument was designed to be portable, battery-powered, and equipped with an extendable measuring head. With appropriate modifications, including adjustments to the measurement wavelength and detection configuration, the system can be adapted to detect alternative refrigerants. While commercially available leak detectors typically offer sensitivities in the range of 3–5 g/year, the developed PA instrument has a significantly higher sensitivity, as it is capable to detect leaks at rates as low as 1.2 g/year.

The measurements yielded the following key results:

- Experiments in a closed small box were conducted to monitor changes in refrigerant gas concentration over time, complemented by finite element simulations using COMSOL Multiphysics. The simulation results closely matched the experimental data, validating their accuracy and allowing for extrapolation to larger environments.
- In an expanded simulation within a 5×4×3 metre room, refrigerant gas concentrations were recorded and isosurface plots were generated to visualise the detection limit concentration front over time. The results illustrated the rapid detectability of the gas and demonstrated the effectiveness of the instrument in a realistic, large-scale setting.
- Controlled leak detection tests confirmed the system's capability to locate leak points precisely and quantify leakage. The PA instrument exhibited fast response times, a wide dynamic concentration range, and high sensitivity, making it a promising tool for refrigerant leak detection.

## References

- [1] S.A. Montzka, J.H. Butler, J.W. Elkins, T.M. Thompson, A.D. Clarke, L.T. Lock, Present and future trends in the atmospheric burden of ozone-depleting halogens, *Nature* 398 (1999) 690–694. <https://doi.org/10.1038/19499>.
- [2] IPCC, ed., *Climate Change 2022 - Mitigation of Climate Change: Working Group III Contribution to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*, 1st ed., Cambridge University Press, 2023. <https://doi.org/10.1017/9781009157926>.

# ASPIRE: An airborne QCLAS for atmospheric water vapor isotopologue measurements

Alex Weitnauer<sup>1,2</sup>, Lorenz Heilmann<sup>1</sup>, Philipp Scheidegger<sup>1</sup>, Lukas Emmenegger<sup>1</sup>, Dominik Brunner<sup>1,2</sup>, Béla Tuzson<sup>1</sup>

1. Empa, Laboratory for Air Pollution / Environmental Technology, 8600 Dübendorf, Switzerland

2. ETH Zürich, Institute for Atmospheric and Climate Science, 8092 Zürich, Switzerland

**Short abstract:** The design and development of a compact airborne LAS targeting water vapor isotopologues in the upper atmosphere is presented. Our approach employs a QCL at 7.35  $\mu\text{m}$  and relies on a novel concept of a circular MPC with an optical path length of 250 m.

Water vapor is the main natural greenhouse gas (GHG) and is significantly influencing atmospheric dynamics. Critical open questions regarding the water vapor budget in the upper troposphere and lower stratosphere (UTLS) could be answered by measuring the isotopic composition of the water vapor. Despite the large potential of such measurements, the availability of in-situ data is still very limited due to a lack of adequate analytical tools. Thus, we propose ASPIRE, a mobile laser absorption spectrometer (LAS) for airborne in-situ measurements of water vapor isotopologues up to the UTLS region, leveraging on our recent advances in balloon-borne instruments [1, 2].

Based on a comprehensive survey of the mid-infrared range, a highly promising spectral window around 7.35  $\mu\text{m}$  (1359  $\text{cm}^{-1}$ ) containing spectral lines of  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{18}\text{O}$ , and HDO with comparable line intensity was identified. Currently, a benchtop setup including a 76 m optical pathlength (OPL) astigmatic Herriot cell is used to determine the optimal spectroscopic parameters and expected performance. Calibration gases covering the typical upper atmospheric conditions are produced by dynamically vaporizing liquid water to produce water vapor mixing ratios in synthetic air from 10000 ppm down to 20 ppm. The isotope ratio measurements ( $\delta\text{H}$  and  $\delta^{18}\text{O}$ ) and their correlation with pressure and  $\text{H}_2\text{O}$  amount fraction will be presented.

Furthermore, to extend the coverage for isotope ratio measurements to higher altitudes, we are redesigning the circular multipass cell [3] by including two individually tilted segments to extend the OPL by more than one order of magnitude without changing its physical dimensions [4]. Raytracing simulations and laboratory tests have shown that this can be achieved while keeping the robustness and low weight needed for balloon-borne applications.

Ultimately, our concept should provide an easy-to-deploy tool for isotope-resolved water vapor profiles at high spatio-temporal resolution.

## References

- [1] M. Graf, P. Scheidegger, A. Kupferschmid, H. Looser, T. Peter, R. Dirksen, L. Emmenegger, and B. Tuzson, "Compact and lightweight mid-infrared laser spectrometer for balloon-borne water vapor measurements in the UTLS", *Atmos. Meas. Tech.*, **14**(2), 1365-1378 (2021).
- [2] S. Brunamonti, M. Graf, T. Bühlmann, C. Pascale, I. Ilak, L. Emmenegger, and B. Tuzson, "SI-traceable validation of a laser spectrometer for balloon-borne measurements of water vapor in the upper atmosphere", *Atmo. Meas. Tech.*, **16**(19), 4391-4407 (2023).
- [3] M. Graf, L. Emmenegger, and B. Tuzson, "Compact, circular, and optically stable multipass cell for mobile laser absorption spectroscopy", *Opt. Lett.* **43**, 2434–2437 (2018).
- [4] L. Heilmann, M. Graf, A. Weitnauer, L. Emmenegger, and B. Tuzson, "Extending the optical path of segmented circular multipass cells by reiteration of reflection patterns", submitted to *Opt. Lett.* (2025).

# Quartz Tuning Fork Front-end Circuits and Optimal Laser Modulation Frequency in QEPAS Sensors

Vincenzina Zecchino<sup>1</sup>, Luigi Lombardi<sup>2</sup>, Cristoforo Marzocca<sup>3</sup>, Giansergio Menduni<sup>1</sup>, Angelo Sampaolo<sup>1</sup>, Vincenzo Spagnolo<sup>1</sup>

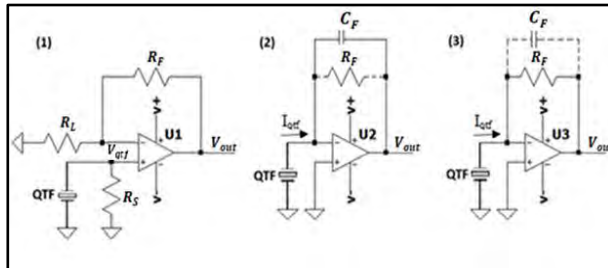
1. PolySense Lab, Dipartimento Interateneo di Fisica, University and Politecnico of Bari, Via Amendola 173, Bari 70126, Italy;

2. PolySenSe Innovations s.r.l, Via Giovanni Amendola 173, 70126 Bari, Italy;

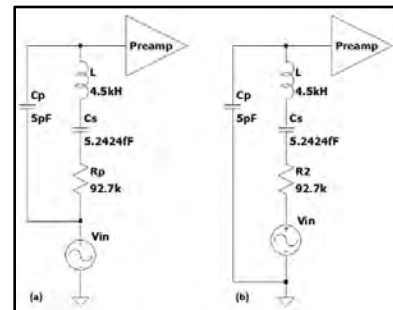
3. Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, Via Orabona 4, 70125 Bari, Italy.

**Short abstract:** This work enhances QEPAS-based gas sensing by showing how front-end circuits impact on finding the optimal laser modulation frequency. Accurate modeling of the quartz tuning fork enables reliable simulations and performance optimization, crucial for achieving detection limits in the sub-ppm and ppb range across various sensing applications.

In Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS), a modulated laser excites a target gas, generating acoustic waves that are detected by a resonant piezoelectric sensor, the quartz tuning fork (QTF). To fully exploit the high quality factor and resonance properties of the QTF, it is essential to operate the system at the optimal modulation frequency, which maximizes the signal-to-noise ratio. This frequency is often estimated through electrical characterization, exciting the QTF with a sinusoidal signal and identifying the frequency which corresponds to the resonance peak. However, experimental evidence shows that this approach does not always yield the true optimal operating frequency for QEPAS technique, as the result strongly depends on the front-end circuit used to read out the QTF signal. To address this issue, the work investigates how different front-end configurations [1-4], shown in Fig. 1, affect the resonance behavior, with the goal of minimizing the mismatch between the electrically identified and the actual optimal operating frequency. At the same time, the study aims to validate the electrical model of a custom quartz tuning fork, with a resonance frequency of 12.4 kHz, finding accurate parameters for the well-established Butterworth-Van Dyke (BVD) model, in which the QTF is represented as a motional RLC branch in parallel with a parasitic capacitance, as in Fig. 2. Model parameters are extracted from appropriate measurements and then verified.



**Fig. 1** Basic configurations of preamplifiers studied, used to interface piezoelectric sensors: (1) voltage amplifier; (2) charge amplifier; (3) transimpedance amplifier.



**Fig. 2** Butterworth-Van Dyke model of the QTF coupled to the preamplifier, in case of (a) electrical characterization and (b) normal operation.

Finding the correct parameters for the equivalent circuit of the QTF ensures that simulation results can be trusted for predictive design, thereby accelerating the development cycle and improving end-application performance. Lastly, by combining careful front-end analysis with the accurate model, this work contributes a practical and effective approach to improve the performance of QTF-based sensors, exploiting the resonance properties to the full, in gas detection and beyond. This contribution is particularly relevant as these sensors continue to gain interest in many different fields such as gas sensing, biosensing, industrial process monitoring and agri-food analysis.

## References

- [1] P. Wieczorek, T. Starecki, "A High Sensitivity Preamplifier for Quartz Tuning Forks in QEPAS (Quartz-Enhanced PhotoAcoustic Spectroscopy) Applications," *Sensors*, vol. **17**, no. **11**, pp. 2528 (2017).
- [2] Luigi Lombardi, Gianvito Matarrese, and Cristoforo Marzocca, "Influence of the Gain-Bandwidth of the Front-End Amplifier on the Performance of a QEPAS Sensor," *Acoustics*, vol. **6**, pp. 240–256 (2024).
- [3] Michele Di Gioia, Luigi Lombardi, Cristoforo Marzocca, Gianvito Matarrese, Giansergio Menduni, Pietro Patimisco, and Vincenzo Spagnolo, "Signal-to-Noise Ratio Analysis for the Voltage-Mode Read-Out of Quartz Tuning Forks in QEPAS Applications," *Micromachines*, vol. **14**, no. **3**, pp. 619 (2023).
- [4] Winkowski, M., Stacewicz, T. Low noise, open-source QEPAS system with instrumentation amplifier. *Sci Rep* **9**, 1838 (2019).