

**UNIVERSITÀ DEGLI STUDI DI GENOVA**  
**AREA RICERCA, TRASFERIMENTO TECNOLOGICO E TERZA MISSIONE**

**SERVIZIO RICERCA**  
**SETTORE RICERCA NAZIONALE**

**IL RETTORE**

Vista la Legge 9 maggio 1989, n. 168 - Istituzione del Ministero dell'Università e della ricerca scientifica e tecnologica e ss.mm.ii;

Visto lo Statuto dell'Università degli Studi di Genova;

Visto il Regolamento Generale di Ateneo;

Visto il Regolamento di Ateneo per l'Amministrazione, la Finanza e la Contabilità;

VISTA la legge 7 agosto 1990, n. 241 recante "Nuove norme in materia di procedimento amministrativo e di diritto di accesso ai documenti amministrativi" pubblicata sulla Gazzetta Ufficiale n. 192 del 18/08/1990 e s.m.i.;

VISTO il Decreto del Presidente della Repubblica 28 dicembre 2000, n. 445 (Disposizioni legislative in materia di documentazione amministrativa) e s.m.i.;

VISTO il Decreto Direttoriale MUR n. 341 del 15/03/2022 di emanazione di un Avviso pubblico per la presentazione di Proposte di intervento per la creazione di "Partenariati estesi alle università, ai centri di ricerca, alle aziende per il finanziamento di progetti di ricerca di base" nell'ambito del Piano Nazionale di Ripresa e Resilienza, Missione 4 "Istruzione e ricerca" – Componente 2 "Dalla ricerca all'impresa" – Investimento 1.3, finanziato dall'Unione europea – NextGenerationEU";

VISTO il Decreto Direttoriale MUR n. 1561 dell'11 ottobre 2022 Codice identificativo PE00000021, Acronimo NEST, Titolo "Extended Partnership Network 4 Energy Sustainable Transition" (CUP D33C22001330002) registrato alla Corte dei Conti il 04/11/2022 con prot. n. 2784 e relativi allegati;

CONSIDERATO che l'Università degli Studi di Genova è leader dello Spoke 4, dal titolo "Clean Hydrogen and Final Uses";

CONSIDERATO che gli Spoke possono emanare - nell'ambito dei limiti e con le modalità previste dall'Avviso - "bandi a cascata" finalizzati alla concessione di finanziamenti a soggetti esterni per attività coerenti con il progetto approvato;

VISTA la delibera della seduta del 27 settembre 2023 con cui il Consiglio di Amministrazione dell'Università degli Studi di Genova ha approvato il modello del "Bando a Cascata" per Organismi di Ricerca;

VISTO il Decreto del Direttore Generale n. 5418 del 14 novembre 2023 di nomina del Responsabile del Procedimento;

VISTO il Decreto del Rettore n. 366 del 24 gennaio 2024 di emanazione del Bando a cascata per il



finanziamento di proposte di intervento per attività di ricerca svolte da Organismi di Ricerca nell'ambito del Programma di ricerca "Extended Partnership Network 4 Energy Sustainable Transition – NEST" PE00000021 - SPOKE N. 4 - CUP D33C22001330002 di cui al Decreto direttoriale n. 1561 del 11 ottobre 2022, registrato dalla Corte dei Conti il 04/11/2022 n. 2784;

CONSIDERATO che alla data di scadenza per la presentazione delle proposte progettuali, fissata entro e non oltre il giorno 29 febbraio 2024, per la **Tematica D - Development of sensors for the detection of impurities in hydrogen** era pervenuta a mezzo PEC all'indirizzo air3@pec.unige.it la seguente proposta:

**PROPONENTE: Università degli Studi di Bari Aldo Moro - Prot. 13319 del 22.02.24**

**TITOLO PROPOSTA: Development of a Hydrogen Impurity Gas Analyzer based on quartz-enhanced photoacoustic Spectroscopy – HIGAS**

TENUTO CONTO che con D.D. 1264 del 18 marzo 2024 la Responsabile del procedimento, Ing. Patrizia Cepollina, ha ritenuto ricevibile, ammissibile e conforme la proposta sopra citata;

CONSIDERATO che nel Bando è previsto che la valutazione di merito tecnico-scientifico dei progetti pervenuti sia affidata ad una Commissione composta da almeno tre esperti esterni al Partenariato, indipendenti e competenti dell'Area tematica dello Spoke;

VISTO il D.R. 1025 del 28 febbraio 2024 di emanazione dell'Avviso di manifestazione di interesse per la costituzione di un Albo di esperti indipendenti a supporto della valutazione di merito dei progetti PNRR presentati sui bandi a cascata del progetto NEST – "Extended Partnership Network 4 Energy Sustainable Transition";

VISTO il D.R. n. 1477 del 26 marzo 2024 che ha costituito l'Albo a supporto della valutazione dei progetti presentati in risposta al bando a cascata, emanato dall'Università degli Studi di Genova in qualità di Leader dello Spoke 4 del progetto NEST – CUP D33C22001330002, con D.R. n. 366 del 24/01/2024;

VISTO il D.R. n. 1549 del 28 marzo 2024 con cui è stata nominata la Commissione di valutazione delle proposte pervenute in risposta al bando a cascata indicato nelle premesse del presente decreto;

ACQUISITO il verbale della Commissione di Valutazione della seduta del 17 maggio 2024 (Prot. 43779 del 20 maggio 2024) per la Tematica D - Development of sensors for the detection of impurities in hydrogen;

VISTO il verbale della riunione del 21 maggio 2024 (Prot. 45085 del 22 maggio 2024) di presa d'atto dei Verbali della Commissione di valutazione;

TENUTO CONTO che in data 27 maggio 2024 è stata inviata all'Università degli Studi di Bari Aldo Moro la comunicazione Prot. 46768 in cui si rendevano noti gli esiti della procedura e si richiedeva la documentazione propedeutica all'adozione del provvedimento di ammissione del finanziamento;



TENUTO CONTO che la documentazione, ricevuta con nota Prot. 52544 del 10 giugno 2024 è stata ritenuta conforme a quanto previsto nel bando a cascata di cui al Decreto del Rettore n. 366 del 24 gennaio 2024, indicato nelle premesse del presente decreto,

#### DECRETA

#### ART. 1

L'ammissione a finanziamento del progetto "Development of a Hydrogen Impurity Gas Analyzer based on quartz-enhanced photoacoustic Spectroscopy – HIGAS" per la **Tematica D - Development of sensors for the detection of impurities in hydrogen** con soggetto proponente Università degli Studi di Bari Aldo Moro - come rappresentato negli Allegati B e C alla proposta presentata con domanda di partecipazione Prot. 13319 del 22 febbraio 2024

#### ART. 2

L'entità dell'agevolazione concessa, a fondo perduto, ammonta a 150.000 euro complessivi come rappresentati nell'allegato C alla proposta presentata con domanda di partecipazione Prot. 13319 del 22 febbraio 2024. L'agevolazione è pari al 100% dei costi di progetto trattandosi di attività di ricerca fondamentale per Organismi di Ricerca. L'agevolazione è concessa a valere sui fondi PNRR - Programma "NEST – Extended Partnership Network 4 Energy Sustainable Transition" Codice PE00000021 finanziato dalla Missione 4, Componente 2, Investimento 1.3, ai sensi del Decreto Direttoriale N. 1561 del 11 ottobre 2022, registrato dalla Corte dei Conti il 04/11/2022 n. 2784 iscritto al Bilancio di Ateneo sul progetto UGOV 100025-2022-LM-PNRR-PE\_NEST\_B\_C\_RICERCA\_DIP (CUP D33C22001330002);

#### ART. 3

Le attività di realizzazione del progetto, come indicate dettagliatamente negli Allegati B e C alla domanda di finanziamento, non potranno essere superiori a 12 mesi a decorrere dalla data di sottoscrizione del Contratto, salvo quanto previsto all'art. 6.3 del bando.

Le attività dovranno comunque essere concluse entro e non oltre il 31 agosto 2025, salvo proroghe del Programma di ricerca NEST concesse dal MUR, affinché siano rendicontate in tempo utile per consentire la chiusura del Programma di ricerca NEST il cui termine è attualmente previsto al 31 ottobre 2025.

#### ART. 4

Il presente atto sarà pubblicato sul sito UniGe <https://unige.it/progetti-finanziati-dal-pnrr> e sul sito <https://fondazionenest.it> - sezione Bandi.

Il documento informatico originale sottoscritto con firma digitale sarà conservato presso l'Area Ricerca, Trasferimento Tecnologico e Terza Missione.

IL RETTORE

Prof. Federico DELFINO

*(documento firmato digitalmente)*



ALLEGATO B

PE00000021

“PNRR MUR - M4C2 – NEST - Extended Partnership  
Network 4 Energy Sustainable Transition”

SPOKE N. 4

CUP D33C22001330002

Research proposal

Development of sensors for the detection of  
impurities in hydrogen

HIGAS - Development of a Hydrogen Impurity Gas  
Analyzer based on quartz-enhanced photoacoustic  
Spectroscopy

- Università degli Studi di Bari Aldo Moro - Physics Department
- Dr. Andrea Zifarelli (PI); Prof. Pietro Patimisco (co-PI)
- Proposal duration in months: 12

<i>ROLE IN THE PROJECT</i>	<i>NAME</i>	<i>SURNAME</i>	<i>INSTITUTION/ DEPARTMENT</i>	<i>QUALIFICATION</i>	<i>YOUNG (under 40 al 31.12.2023)</i>	<i>F/M</i>
Principal Investigator	<i>Andrea</i>	<i>Zifarelli</i>	<i>Physics Department - University of Bari</i>	<i>RTD-A Researcher</i>	<i>Yes</i>	<i>M</i>
co-Principal Investigator (PI)	<i>Pietro</i>	<i>Patimisco</i>	<i>Physics Department - University of Bari</i>	<i>Associate Professor</i>	<i>Yes</i>	<i>M</i>
Team Member	<i>Mariagrazia</i>	<i>Olivieri</i>	<i>Physics Department - University of Bari</i>	<i>Ph.D. Student</i>	<i>Yes</i>	<i>F</i>
Team Member	<i>Aldo Francesco Pio</i>	<i>Cantatore</i>	<i>Physics Department - University of Bari</i>	<i>Ph.D. Student</i>	<i>Yes</i>	<i>M</i>

## ABSTRACT

The HIGAS project aims at developing an innovative platform for detection of impurities in hydrogen employing quartz-enhanced photoacoustic spectroscopy as sensing technique. The development of hydrogen-related technologies for clean energy production and storage has encountered the obstacles related to the presence of trace contaminants in the hydrogen matrices, strongly affecting the performances of fuel cell systems. Nowadays, the detection and analysis of these impurities is mainly performed employing gas chromatography techniques coupled with different types of detectors. This instrumentation is expensive, characterised by a large footprint and not capable of real-time monitoring. A promising alternative is represented by optical absorption spectroscopy. Among the different techniques, quartz-enhanced photoacoustic spectroscopy (QEPAS) has demonstrated the capability to perform trace gas detection for environmental monitoring with excellent sensitivity and selectivity, also providing high sensor compactness and ruggedness. The QEPAS sensors exploit a quartz tuning fork as resonant piezoelectric transducer to convert the photoacoustic waves generated by the interaction among a laser source and the target molecule into an electric signal proportional to the target concentration. The tuning fork is typically coupled to millimetric resonator tubes in the so-called QEPAS spectrophone. In this project, two of the most relevant impurities in hydrogen samples will be investigated, namely carbon monoxide and ammonia. First, the spectral features of the two analytes to be targeted will be individuated and the response of the QEPAS spectrophone in the hydrogen matrix will be characterised. Then, two QEPAS sensors will be assembled, one for each analyte, identifying the best components with the aim of developing a shoe-size QEPAS box capable of standalone operation. Finally, the sensors will be tested and the performances in terms of detection limits will be assessed.

## RESEARCH PROPOSAL

Sections (a) and (b) should not exceed 4 pages. References do not count towards the page limits.

### Section a. State-of-the-art and objectives

The challenge of reducing the effects of global climate change must involve the path towards the reduction of carbon emission. In this perspective, a strong cut in the use of carbon-emitting energy sources (coal, oil, etc.) would lead to a global benefit. An important alternative to coal and fossil fuels is represented by hydrogen-related technologies, where hydrogen is used as an energy vector to power fuel cell systems and produce electrical energy starting from electrochemical oxidation of hydrogen. Different approaches have been investigated, such as polymer electrolyte fuel cells (PEFCs) and proton exchange membrane fuel cells (PEMFCs) [1-2]. Nevertheless, this technology is not competitive with traditional internal combustion engines due to the strict requirement of pure or purified hydrogen, whose preparation and storage costs are still high. The impurities are generated in the hydrogen production process, such as natural gas steam reforming in which the steam reacts with the natural gas in a set of reactions to produce mainly hydrogen, carbon dioxide, and carbon monoxide [3]. The need for high-purity hydrogen comes from the impact of impurities in the hydrogen matrix on the lifetime of the fuel cell systems, as even trace concentrations of contaminants may lead to relevant degradation of the fuel cell catalyst [4]. The list of damaging impurities in hydrogen includes: carbon monoxide, ammonia, carbon dioxide, sulphur compounds, and hydrocarbons. The analytes concentration in the hydrogen matrix is strongly dependent on the hydrogen production method; however these contaminants could significantly affect the fuel cell systems operations at concentration level in the range of part-per-million (ppm) and below. Therefore, it is crucial to adopt sensitive and accurate detection methods for online and offline detection of contaminants in hydrogen, to fulfil the requirements of international standards (ISO 14687:2019) [5].

Carbon monoxide (CO) represents a threat for hydrogen fuel cells due to its capability of binding to platinum (Pt) anodes, which are widely employed in fuel cells for hydrogen oxidation reactions and oxygen reduction reactions in acidic environments. For instance, a voltage loss of 85% was observed in a PEMFC cell following an exposure of 70 ppm for 6 hours [6], and the need for a constant concentration of CO below 10 ppm has been reported [7]. ISO 14687:2019 requires a CO threshold concentration of 0.2 ppm for grade D applications (fuel cells for road vehicles). Ammonia (NH<sub>3</sub>) is a danger for fuel cell systems due to its reactive nature affecting the ion exchange capacity of the fuel cell leading to irreversible damage for high concentration or prolonged exposure [8]. ISO 14687:2019 requires a NH<sub>3</sub> threshold concentration of 0.1 ppm for grade D applications.

With the aim of monitoring the concentrations of hydrogen impurities different detection methods have been developed, for both offline and online monitoring. In the first case, the hydrogen mixtures are sampled and then delivered to a laboratory facility to be analysed. The detection and quantification of contaminants is performed employing instrumentation characterised by high sensitivity and selectivity, which in turn is usually expensive, requiring large footprint and qualified users. In this field, the golden standard is represented by gas chromatography coupled with different kinds of detectors as mass spectrometers, flame ionisation, and pulsed discharge helium ionisation detectors (PDHID) [9].

Conversely, online monitoring techniques allow the detection and quantification of hydrogen impurities on field and in real time. These methods represent a crucial tool to monitor contaminants' concentrations continuously, thus providing a prompt response in case of unexpected increase in impurities levels preventing malfunctioning of the apparatus. In this field, optical-based techniques may represent reliable solutions, being capable of sensitive detection for online monitoring. Sensors based on Fourier Transform InfraRed (FTIR) spectroscopy [10], cavity-enhanced Raman spectroscopy [11], and photoacoustic spectroscopy [12] for hydrogen contaminants detection have been demonstrated. However, the rising interest for hydrogen-related

technologies has nowadays pushed new efforts in the development of sensitive, compact, rugged and reliable optical sensors for contaminants detection in hydrogen matrix.

In this project, we aim to develop a new sensing platform for two of the most relevant impurities in hydrogen matrices, i.e., CO and NH<sub>3</sub>, based on quartz-enhanced photoacoustic spectroscopy (QEPAS). The latter represents a development of traditional photoacoustic spectroscopy, which has demonstrated higher sensitivity in a more compact sensing system [13]. Two different QEPAS sensors will be developed, each one housed inside a portable, shoe-size box equipped with the electronic boards and the gas line management system required to allow standalone operations. The goal of the project is to transfer the technologies developed for environmental monitoring in atmosphere (nitrogen matrix) to the detection of impurities in hydrogen, thus providing custom solutions ad hoc for this gaseous matrix. The QEPAS sensor will be validated in a laboratory environment, demonstrating their capabilities to match the requirements needed by the industry for fuel cell systems safety.

## Section b. Methodology

Photonics sensors based on laser absorption spectroscopy (LAS) are of growing interest due to the recent development of powerful lasers tunable over large-wavelength ranges which permits unambiguous detection of numerous substances at low concentrations and in many cases even calibration free operation. They are considerably faster than non-photonics sensors (e.g. wet-chemical or chromatographic apparatus) and suffer from minimal drift. Photonics offers high specificity and sensitivity for real time in-situ measurement and allows the contactless simultaneous detection of many substances [14]. Photoacoustic spectroscopy follows different rules to absorption spectroscopy based on Lambert-Beer optical absorption, providing greater compactness and lower costs. The absorption of infrared photons in a gas sample results in the excitation of molecular energy levels whose energy is released as heat. The generated signal is proportional to the incident light intensity and, should this intensity be modulated, localised transient heating results. The medium responds creating acoustic (pressure) waves [15].

PAS sensors use a microphone to detect the pressure wave in a resonant acoustic gas cell. QEPAS replaces the microphone with a spectrophone, composed by a quartz-tuning fork (QTF) and a pair of millimetre-size resonator tubes, aligned on both sides of the QTF in a way that the laser beam can be focused between the QTF prongs while passing through both tubes [13]. A schematic of the QEPAS spectrophone is shown in Fig. 1a. When the laser beam is modulated at the resonance frequency of the QTF or a subharmonic, a standing wave vibrational pattern is created within the resonator tubes which deflects the two prongs in opposite directions, exciting the QTF in a piezoelectrically-active, anti-symmetrical flexural mode. Thus, an electrical signal proportional to the absorbing analyte concentration is generated. Thus, the technique is baseline free, greatly easing calibration with respect to absorption spectroscopy. The main strengths of QEPAS are: immunity to environmental acoustic noise (an issue for standard PAS systems), no requirement for optical detectors, compactness, capability to analyse small gas samples, wavelength-insensitivity, hyperspectrality, high accuracy and sensitivity, very large linear dynamic range (from few % to part per trillion range), long-time stability, low-cost and able to operate in real time and in situ [16].

From 2002, several QEPAS sensors in laboratory prototype system have been developed and more than 30 different analytes have been detected using a wide range of laser sources, from UV-visible (LEDs) to near-IR (diode) and mid-IR range (ICLs and QCLs), up to Terahertz range (QCLs). In most cases, ultimate detection limits in the part-per-billion range and down to part-per-trillion have been achieved, as shown in Fig. 1b [17].

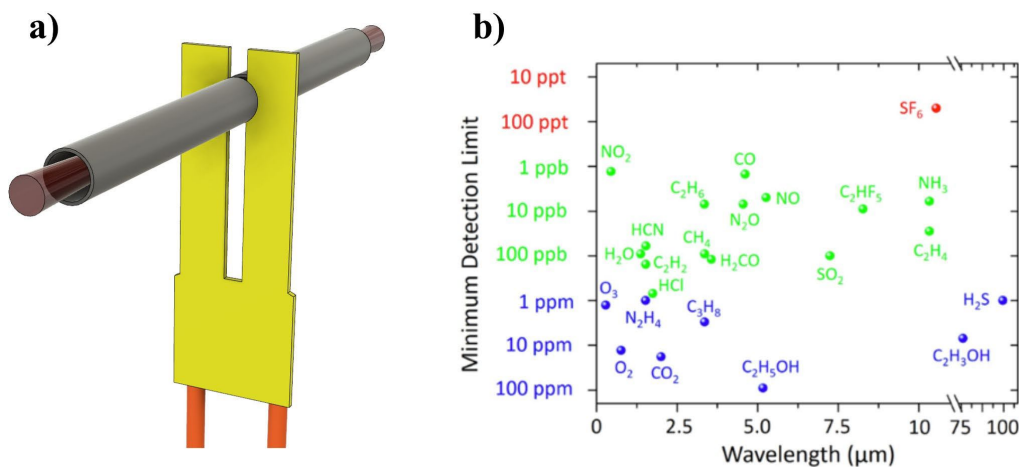


Figure 1. (a) Schematic of the QEPAS spectrophone consisting of a QTF (yellow) and a pair of millimetric resonator tubes (grey). The laser beam (transparent red) is focused through the tubes between the QTF prongs. (b) QEPAS detection limits for a selected list of gas species [17].

Prior to 2013, all the QEPAS sensors reported in the literature employed commercial standard quartz tuning forks (QTFs) (i.e. those used in watches) operating at the fundamental flexural resonance mode with a frequency of  $\sim 32.7$  kHz, which size and geometry has been optimised for timing and not for sensing. Indeed, the prongs spacing ( $300 \mu\text{m}$ ) and the micro-resonator tubes (internal diameter of  $600 \mu\text{m}$ ) are very narrow, making difficult the optical coupling with the laser source. Additionally, the operating frequency of  $32.7$  kHz is too high with respect to the energy relaxation processes occurring in the absorbing gas, resulting in low radiation-to-sound conversion efficiency. The development of custom QTF led to a key breakthrough represented by custom tuning forks with (i) reduced resonance frequency while keeping the quality factor high and (ii) enlarged prong spacing. Compared to the original design, the new tuning forks result in better sensing performance [18].

Hydrogen represents an excellent gaseous matrix for absorption spectroscopy, being mainly transparent in the IR region with the exception of some weak absorption lines around  $2.12 \mu\text{m}$  [19]. Therefore, the optical detection can be performed by choosing suitable laser sources capable of matching spectral lines of target gases presenting no spectral interference with the absorption spectrum of other contaminants. In this way, the maximum spectroscopic signal will be found by means of a simple scan of the laser wavelength, thus avoiding the use for expensive reference cells but ensuring high selectivity to the measurements.

Moreover, from the perspective of photoacoustic waves generation, hydrogen would provide several benefits with respect to nitrogen or standard air. The change in the gas matrix leads to a change in the energy dissipation mechanism occurring in a vibrating prong, which is the damping by the surrounding fluid [20]. As a result, the matrix composition and its thermodynamic parameters affect the QTF quality factor. Since the QEPAS signal is proportional to the QTF quality factor, the ultimate sensor sensitivity will be in turn affected by the selected matrix [21]. For gas matrices composed by molecules with low molecular weight, such as hydrogen, an increase in the QTFs' quality factor is expected, thus resulting in an overall improvement of the detection performances. Nevertheless, to fully exploit the benefit arising from the hydrogen matrix, it is mandatory to use custom QEPAS spectrophone, with QTF geometry and resonator tubes size tailored to enhance the sensing performances.



## Reference

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### Section c. Available instrumentations and resources

The Physics Department of University of Bari contains the main equipment and tools to realise, test and validate Quartz-Enhanced Photoacoustic Sensing Systems for trace gas detection. This includes:

- a machine shop for the realisation of mechanical parts of vast complexity in three dimensions
- a 3D-printer for produce custom components with remarkable flexibility
- state-of-the-art facilities for design and realisation of acoustic detection modules
- testing workbenches for the characterization of optoacoustic transducers
- a clean room (80 m<sup>2</sup>) equipped with mask aligner, e-beam evaporator, rapid thermal annealer and microscopes for realising electrical contacts on quartz crystals.
- several quantum cascade lasers and interband laser sources operating in the mid-infrared as well as several diode laser sources
- an optical spectrum analyzer for the characterization of laser sources
- an FT-IR spectrometer for gas molecules characterization
- several sets of THORLABS optics for the near- and mid-infrared spectral range
- gas management system, including over 20 gas flow lines for toxic/corrosive analytes, with flow and pressure controllers, vacuum systems, gas cabinets and cylinders with certified gas mixtures.

### Section d. GANTT diagram

For scientific and technological effectiveness, the proposed project activities will be developed into 4 separate work packages (WPs), with clearly identified schedules (Gantt chart in Fig. 2)

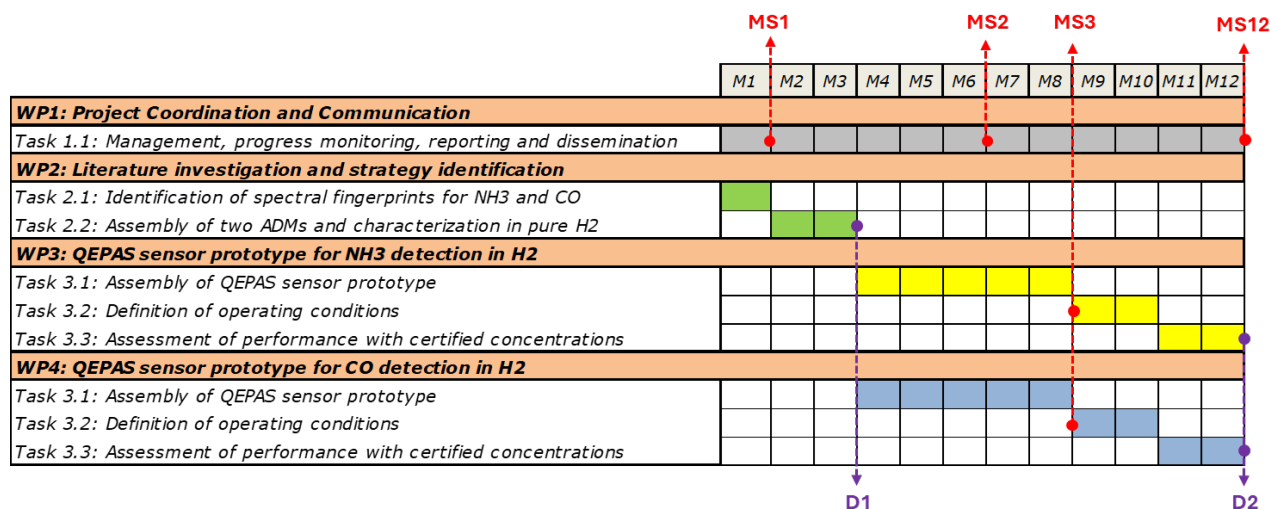


Figure 2. Gantt chart of the project.

Timing of the project is indicated in one-month packages in a Gantt Chart, broken down by work packages and tasks, including milestones and deliverables.

#### WP1 – Project Coordination and Communication

Task 1.1: Management, progress monitoring, reporting and dissemination (M1-M12)

The scientific activities will include: tracking progress towards scientific deliverables and milestones; making decisions on scientific activities in order to implement the overall strategy; drafting technical reports; creating a broad dissemination of communications.

#### WP2 – Literature investigation and strategy identification

Task 2.1: Identification of spectral fingerprints for NH3 and CO (M1)

This task will be devoted to the reconstruction of the infrared spectrum absorption of two selected analytes, namely CO and NH3, based on publicly available databases, including HITRAN, PNNL, Biorad, NIST, and SDDBS. This literature research will be used as a guideline for the selection of the well-resolved features that can be used as fingerprints of related molecules, simplifying the identification process especially with interferers.

Task 2.2: Assembly of two ADMs and characterization in pure H2 (M2-M3)

Spectrophones composed by a custom quartz tuning fork (QTF) and a pair of resonator tubes will be assembled in aluminium Acoustic Detection Module (ADM). The resonance properties of the spectrophone (the resonance frequency and its quality factor) as well as the noise level will be measured in pure hydrogen and compared with the performance in air.

#### WP3 – QEPAS sensor prototype for NH3 detection in H2

Task 3.1: Assembly of QEPAS sensor prototype (M4-M8)

In this task, the QEPAS sensor system for NH<sub>3</sub> detection in H<sub>2</sub> will be assembled starting from components, including the mechanical, optical and electrical parts. The laser source will be optically coupled with the ADM by means of a focusing lens. The prototype will include electronic control boards for controlling the laser source and a transimpedance amplifier for processing the QTF signal. The table-top QEPAS system will have full functionality, including gas management system, control and communications with a laptop.

#### Task 3.2: Definition of operating conditions (M9-M10)

The operating conditions will be assessed. The best operating pressure maximising the signal-to-noise ratio will be found. The wavelength modulation and second harmonic detection technique, together with an advanced data analysis and fitting models, will be implemented in order to retrieve the concentration measurement of the NH<sub>3</sub> in the H<sub>2</sub> matrix.

#### Task 3.3: Assessment of performance with certified concentrations (M11-M12)

The QEPAS sensor prototype will be tested in a laboratory environment using certified reference gas cylinders of NH<sub>3</sub>/H<sub>2</sub> mixture and a gas mixing device. The test will be performed in a controlled environment, with specific parameters regulated, including temperature, humidity, pressure and gas flow. The performance of the sensor in terms of sensitivity, ultimate detection limit and long-term stability will be assessed.

### *WP4 – QEPAS sensor prototype for CO detection in H<sub>2</sub>*

#### Task 4.1: Assembly of QEPAS sensor prototype (M4-M8)

In this task, the QEPAS sensor system for CO detection in H<sub>2</sub> will be assembled starting from components, including the mechanical, optical and electrical parts. The laser source will be optically coupled with the ADM by means of a focusing lens. The prototype will include electronic control boards for controlling the laser source and a transimpedance amplifier for processing the QTF signal. The table-top QEPAS system will have full functionality, including gas management system, control and communications with a laptop.

#### Task 4.2: Definition of operating conditions (M9-M10)

The operating conditions will be assessed. The best operating pressure maximising the signal-to-noise ratio will be found. The wavelength modulation and second harmonic detection technique, together with an advanced data analysis and fitting models, will be implemented in order to retrieve the concentration measurement of the CO in the H<sub>2</sub> matrix.

#### Task 4.3: Assessment of performance with certified concentrations (M11-M12)

The QEPAS sensor prototype will be tested in a laboratory environment using certified reference gas cylinders of CO/H<sub>2</sub> mixture and a gas mixing device. The test will be performed in a controlled environment, with specific parameters regulated, including temperature, humidity, pressure and gas flow. The performance of the sensor in terms of sensitivity, ultimate detection limit and long-term stability will be assessed.

### **Section e. Milestones, Deliverables and KPI**

The list of Milestones is reported in Table 1.

Table 1. List of Milestones

MS	Milestone Title	WP	Due	Means of Verification
<b>MS1</b>	Definition of strategy	1	M1	Report on dissemination plan and schedule of scientific activities
<b>MS2</b>	Mid-Term Project Status	1	M6	Report on mid-term progresses related to scientific activities and assessment of strategies for next activities
<b>MS3</b>	Assembly of two QEPAS sensors	3-4	M8	Report on the design and realisation of a QEPAS sensor prototype for NH <sub>3</sub> detection in H2 and a QEPAS sensor prototype for CO detection in H2
<b>MS4</b>	Communication and dissemination reached	1	M12	Report on dissemination to the scientific community (open-access publications, scientific seminars and conferences) and to a wider public (social media, local and national press release)

The list of Deliverables is reported in Table 2.

Table 2. List of Deliverables

D	Deliverable Title	WP	Due	Type
<b>D1</b>	Report on laser characteristics and on performance of spectrophone in H <sub>2</sub> environment	2	M3	Report

<b>D2</b>	A QEPAS sensor prototype for NH <sub>3</sub> detection in N <sub>2</sub> and a QEPAS sensor prototype for CO detection in N <sub>2</sub>	3-4	M12	Two Demonstrators with datasheet/specification
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## Annexes: Curriculum vitae research team

### Curriculum vitae PI

#### PERSONAL INFORMATION

Family name, First name: ZIFARELLI, ANDREA

Researcher unique identifier(s): ORCID: 0000-0003-1875-4671; SCOPUS Author ID: 57204418400

Date of birth:

Nationality:

URL for website: <http://polysense.poliba.it/index.php/andrea-zifarelli/>

#### · EDUCATION

- |      |  |
|------|--|
| 2022 | PhD in Physics<br>Physics Department, Università degli Studi di Bari “Aldo Moro”, Italy<br>Supervisor: Prof. Vincenzo Spagnolo, Prof. Pietro Patimisco |
| 2018 | Master of Science in Physics<br>Physics Department, Università degli Studi di Bari “Aldo Moro”, Italy  |

#### · CURRENT POSITION(S)

- |        |   |
|--------|---|
| 2023 – | RTD-A researcher<br>Physics Department, Università degli Studi di Bari “Aldo Moro”, Italy |
|--------|---|

#### · PREVIOUS POSITIONS

- |             |  |
|-------------|--|
| 2022 – 2023 | Post-Doc Researcher (assegnista di ricerca)<br>Physics Department, Università degli Studi di Bari “Aldo Moro”, Italy |
|-------------|--|

#### · FELLOWSHIPS AND AWARDS

- |      |   |
|------|---|
| 2022 | Post-Doctoral Research Fellowship<br>Spectroscopy Research and Development Group, THORLABS GmbH,<br>Bergkirchen, Germany  |
| 2021 | Best Presentation Award, International School of Quantum Electronics, 64 <sup>th</sup><br>course, Progress in Photoacoustic and Photothermal Phenomena                    |
| 2019 | Visiting Researcher at Institute of Laser Spectroscopy in Shanxi University,<br>Taiyuan, China, within the “Hundred Talents” project of the Chinese<br>Academy of Science |

#### · SUPERVISION OF GRADUATE STUDENTS

- 2023 – n°1 PhD Students  
Interuniversity PhD course in Smart and Sustainable Industry, Technical University of Bari, Italy
- 2023 – n°2 Master Students  
Master's degree in Physics, Physics Department, Università degli Studi di Bari, Italy

#### · ORGANISATION OF SCIENTIFIC MEETINGS

- 2023 Organiser of CONFERENCE ON PHOTONICS FOR ADVANCED SPECTROSCOPY AND SENSING / Italy  
International Conference/ 150 participants / Italy  
<https://www.c-pass.eu/>

#### · REVIEWING ACTIVITIES

- 2023– Guest Editor of the Special Issue of “Sensors” journal, MDPI: “Photonics for Advanced Spectroscopy and Sensing”  
[https://www.mdpi.com/journal/sensors/special\\_issues/9533LV9TQ9](https://www.mdpi.com/journal/sensors/special_issues/9533LV9TQ9)
- 2023 – Review Editor of the section “Environmental Analytical Methods” of “Frontiers in Environmental Chemistry” journal, Frontiers In  
<https://www.frontiersin.org/journals/environmentalchemistry/sections/environmental-analytical-methods/editors>
- 2023 – Topic Coordinator of the Special Issue of “Frontiers in Chemistry” journal, Frontiers In: “Recent Advances in Optical Sensing for Multi-Gas Detection”  
<https://www.frontiersin.org/research-topics/56166/recentadvances-in-optical-sensing-for-multi-gas-detection>

#### · MAJOR COLLABORATIONS

Lei Dong and Hongpeng Wu, *Development of optical sensors based on light-induced thermoelastic spectroscopy*, Shanxi University, State Key Laboratory of Quantum Optics and Quantum Optics Devices, Taiyuan, China  
Reference Paper: <https://doi.org/10.1063/5.0062415>

T. Muller, *Multivariate analysis and digital twin modelling: alternative approaches to molecular relaxation in photoacoustic spectroscopy*, Regensburg University of Applied Sciences, Regensburg, Germany  
Reference Paper: <https://doi.org/10.1016/j.pacs.2023.100564>

M. Gonzalez, *Hydrocarbons monitoring for natural gas analysis using optical spectroscopy*, Aramco Services Company, Aramco Research Center, Houston, United States  
Reference Paper: <https://doi.org/10.1016/j.pacs.2023.100448>



R. Blanchard, *Study of optical sensors based on broadband infrared sources for multi-gas species detection*, Pendar Technologies, Cambridge, United States  
Reference Paper: <https://doi.org/10.1016/j.pacs.2019.100159>

Q.J. Wang, *Development of QEPAS-based sensor box for simultaneous detection of contaminants in atmosphere*, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore  
Reference Paper: <https://doi.org/10.3389/fenvc.2022.926233>

### Current grants

<i>Project Title</i>	<i>Funding source</i>	<i>Amount (Euros)</i>	<i>Period</i>	<i>Role of the PI</i>	<i>Relation to current proposal</i>
-	-	-	-	-	-

## Curriculum vitae CO-PI

### PERSONAL INFORMATION

Family name, First name: PATIMISCO, PIETRO

Researcher unique identifiers: <https://orcid.org/0000-0002-7822-2397>, Scopus Author ID: 54950201900

URL for website: <http://polysense.poliba.it/index.php/pietro-patimisco/>

### · EDUCATION

- |      |   |
|------|---|
| 2013 | PhD in Physics<br>Physics Department, University of Bari, Italy<br><u>PhD Supervisor: Prof. Gaetano Scamarcio</u> |
| 2009 | Master's degree in physics<br>Physics Department, University of Bari, Italy                                       |

### · CURRENT POSITION

- |        |  |
|--------|--|
| 2023 – | Associate Professor (SSD FIS03)<br>Physics Department, University of Bari, Italy |
|--------|--|

### · PREVIOUS POSITIONS

- |             |  |
|-------------|--|
| 2020 – 2023 | Assistant Professor (Ricercatore a Tempo Determinato-b)<br>Physics Department, University of Bari, Italy |
| 2018 – 2020 | Assistant Professor (Ricercatore a Tempo Determinato-a)<br>Technical University of Bari, Italy           |
| 2017 – 2018 | Post-Doc Position<br>Physics Department, University of Bari, Italy                                       |
| 2013 – 2016 | Post-Doc Position<br>Physics Department, University of Bari, Italy                                       |

### · FELLOWSHIP

- |             |  |
|-------------|--|
| 2016 – 2017 | Post-Doctoral Research Fellowship<br>Laser Science Group, Electrical and Computer Engineering Department, Rice<br>University, Houston, Texas |
|-------------|--|

2018 – 2019 Visiting Researcher at Institute of Laser Spectroscopy in Shanxi University, Taiyuan, China, within the “Hundred Talents” project of the Chinese Academy of Science

#### **SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS**

2019 – n°8 Master Students  
Master’s degree in physics, Physics Department, University of Bari, Italy

2020 – n°4 PhD Students  
PhD School in Physics, Physics Department, University of Bari, Italy

2021 – n°2 PhD Students  
Interuniversity PhD School in Industry 4.0, Technical University of Bari, Italy

2021 – n°2 post-Docs  
Physics Department, University of Bari, Italy

#### **ORGANISATION OF SCIENTIFIC MEETINGS**

2023 Organiser and Member of the Technical Committee of CONFERENCE ON PHOTONICS FOR ADVANCED SPECTROSCOPY AND SENSING / Italy International Conference / 150 participants / Italy  
<https://www.c-pass.eu/>

#### **INSTITUTIONAL RESPONSIBILITIES**

2017 - Member of the Technical Committee of Polysense Laboratory  
Technical University of Bari, Italy

2018 – 2020 Member of “Giunta del Dipartimento di Fisica”  
University of Bari, Italy

2019 – 2020 Member of “Consiglio della Scuola di Scienze e Tecnologia”  
University of Bari, Italy

2020 – 2023 Vice-Coordinator of the PhD Program Committee of the Interuniversity PhD School in Industry 4.0  
Technical University of Bari, Italy

2023 – Vice-Coordinator of the PhD Program Committee of PhD School in Physics  
University of Bari, Italy

#### **PATENTS**

2020 - Chinese Patent n° 202010087714.6. Title “*A method and a device for improving the sensitivity of gas concentration detection of quartz enhanced photoacoustic spectrum*”. Inventors: H. Wu, L. Dong, Z. Shang, S. Li, V. Spagnolo, A. Sampaolo, P. Patimisco.

2022 - Chinese Patent n° 112834430B. Title “*A device and method for gas detection based on acoustic pulse excitation of photoacoustic cell*”. Inventors: H. Wu, L. Dong, T. Wei, W. Yinzho, V. Spagnolo, A. Sampaolo, P. Patimisco, M. Giglio.

## REVIEWING ACTIVITIES

2018 – Member of the Editorial Board of “Sensors” journal MDPI, <https://www.mdpi.com/journal/sensors/editors>

2019 – 2020 Guest Editor of the Special Issue of “Sensors” journal, MDPI: Optical Spectroscopy, Sensing, and Imaging from UV to THz Range [https://www.mdpi.com/journal/sensors/special\\_issues/OSSITR](https://www.mdpi.com/journal/sensors/special_issues/OSSITR)

2022 – 2023 Guest Editor of the Special Issue of “Photoacoustic” journal, Elsevier: Photoacoustic spectroscopy for gas sensing: from theoretical modelling to applications <https://www.sciencedirect.com/journal/photoacoustics/special-issue/107XM34RKBJ>

## MAJOR COLLABORATIONS

Simone Borri and Paolo de Natale, *Study and development of cavity-enhanced absorption spectroscopic techniques for highly sensitive and selective trace gas sensing*, Istituto Nazionale di Ottica (INO-CNR), Firenze, Italia.  
Reference Paper: <https://doi.org/10.1016/j.pacs.2022.100436>

Lei Dong and Hongpeng Wu, *Development of optical sensors for real-time and in-situ monitoring of air*, Shanxi University, State Key Laboratory of Quantum Optics and Quantum Optics Devices, Taiyuan, China  
Reference Paper: <https://doi.org/10.1016/j.pacs.2024.100585>

Yufei Ma, *Development of light-induced thermoelastic spectroscopy with custom quartz tuning fork*, National Key Laboratory of Science and Technology on Tunable Laser, Harbin Institute of Technology, Harbin 150001, China  
Reference Paper: <https://doi.org/10.1016/j.pacs.2022.100381>

Frank Tittel, *Development of quartz-enhanced photoacoustic spectroscopy for sensing applications*, Rice University, Department of Electrical and Computer Engineering, Houston, TX, United States  
Reference Paper: <https://doi.org/10.1016/j.pacs.2023.100502>

Y. Bidaux and J. Faist, *Study of wavelength modulation spectroscopy with quantum cascade laser sources*, Eidgenössische Technische Hochschule (ETH), Institute for Quantum Electronics, Zurich, Switzerland  
Reference Paper: <http://dx.doi.org/10.1364/OE.24.025943>

R. Blanchard, *Study of optical sensors based on broadband infrared sources for multi-gas species detection*, Pendar Technologies, Cambridge, United States  
Reference Paper: <https://doi.org/10.1016/j.pacs.2019.100159>

M. Deffenbaugh, *Development of optical sensors for oil/gas applications*, Aramco Services Company, Houston, TX, United States  
Reference Paper: <https://doi.org/10.1016/j.snb.2018.11.132>

### Current grants

<i>Project Title</i>	<i>Funding source</i>	<i>Amount (Euros)</i>	<i>Period</i>	<i>Role of the PI</i>	<i>Relation to current proposal</i>
OPTAPHI	H2020-MSCA-ITN-2019	200 k€	2019 – to date	<ul style="list-style-type: none"> <li>- Responsibility of commercialization</li> <li>- IP manager</li> </ul>	Study of innovative spectroscopic techniques for gas sensing
PASSEPARTOUT	H2020-ICT-37-2020-101016956	630 k€	2020 – to date	<ul style="list-style-type: none"> <li>- Local Unit Manager</li> <li>- WP Leader</li> </ul>	Development of quartz-enhanced photoacoustic sensors for air pollutants detection
NQSTI2022	PNRR Extended Partnerships “National Quantum Science and Technology Institute”	870 k€	2022 – to date	<ul style="list-style-type: none"> <li>- Task Leader</li> </ul>	Development of quantum sensing technologies for gas sensing

AGRITECH2022	PNRR National Research Centre for Agricultural Technologies	80 k€	2022 – to date	- Task Leader	Development of quartz-enhanced photoacoustic sensors for agricultural monitoring applications
QUASIMODO	MUR Dipartimento di Eccellenza 2023-2027	200 k€	2023 – to date	- WP Leader	Quantum Sensing and Modeling for One-Health
SIMBA	PRIN PNRR 2022	50 k€	2023 – to date	- Local Manager Unit - WP Leader	Study of surface acoustic waves on piezoelectric substrates

## ALLEGATO C - Budget personale costi standard



TABELLA COSTI PERSONALE STANDARD				COSTO DEL PERSONALE	TD
FASCIA DI COSTO /LIVELLO	NUMERO SOGGETTI	COSTO ORARIO vedi nota	MONTE ORE		
Basso	0	- €	0	- €	
Medio	1	48 €	150	7.200 €	
Alto	0	- €	0	- €	
TOTALI	1		150	7.200 €	

COSTO ORARIO: si deve far riferimento al Decreto Interministeriale n. 116 del 24/1/2018

*Firma digitale del  
Legale rappresentante del Proponente*



BUDGET DI PROGETTO	COSTO DEL PERSONALE	OVERHEAD	Costi per servizi di Consulenza Specialistica	Costi per licenze direttamente imputabili al progetto	Costi per materiali e attrezzature direttamente imputabili al progetto	Costi per altre tipologie di spese direttamente imputabili al progetto	COSTO TOTALE
Pietro Patimisco	7.200,00 €	1.080,00 €	0,00 €	0,00 €	51.000,00 €	20.000,00 €	79.280,00 €
Andrea Zifarelli	0,00 €	0,00 €	0,00 €	0,00 €	51.000,00 €	19.720,00 €	70.720,00 €
Partecipante ....		0,00 €					0,00 €

Totale

150.000,00 €

Firma digitale del  
Legale rappresentante del Proponente